

ON THE QUANTIZATION AND MEASUREMENT OF MOMENTUM OBSERVABLES

Keith McFarlane

A Thesis Submitted for the Degree of PhD
at the
University of St Andrews



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"On the Quantization and Measurement of Momentum Observables"

a thesis submitted for the
degree of
Doctor of Philosophy
in the
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by
Keith McFarlane

St Leonard's College

April 1980



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Dedication

To my grandparents, Mr and Mrs P. McColl,
for a lifelong support of my ambition and faith
in my ability;

to my fiancée, Miss Margaret Hawkridge,
for past and future happiness; and

to the memory of my friend and mentor, Arthur Bryce,
for his kindness and his appreciation of life.

Acknowledgements

Whereas there is scarcely a member of the Department of Theoretical Physics who has not helped or encouraged me in the composition of this thesis, I nevertheless particularly wish to thank the following:

My supervisor, Dr K.K. Wan, for his energy, enthusiasm, and great sympathy in guiding so volatile a mind on so sober a course;

Dr N.C. McGill, for his most able collaboration in our joint excursions into the General Theory of Relativity;

Professor J.F. Cornwell, for acting as my supervisor during the academic year 1977-'78; and finally

Miss Linda McLean, my typist, whose contribution to this thesis is surely more obvious even than that of the author.

Preface .

This thesis is the outcome of research conducted into the quantization of observables defined over a Riemannian configuration manifold, and is naturally divided into three chapters:

The first chapter is essentially concerned with the development, from physical bases, of the concepts of classical and quantum "global measurability", which, when combined with the requirement that all quantizable momenta shall be either classically or quantum mechanically globally measurable, result in the exclusion from the class of quantizable momenta of all those observables which are not quantizable in accordance with G.W. Mackey's natural procedure. The refinement of exact global measurability is then introduced, and the physically important class of "Killing" momenta are found to be exactly classically and quantum mechanically globally measurable and moreover quantizable by means of Mackey's scheme.

The second chapter seeks to analyse the algebraic structure of the Mackey-quantizable momenta, so as to compare and contrast his geometric scheme with the various algebraic schemes which have frequently been proposed. As an extension of this work, a natural geometric quantization is proposed for the more general class of observables "linear in momentum", the set of quantizable such entities determined, and its algebraic properties discussed. It is concluded that, if Mackey's procedure is, as we argue, correct and exhaustive of the quantizable momenta, then algebraic rules of quantization do not, in general, obtain among the momenta defined over a Riemannian space, though in the case of momenta, such as the Killing momenta, reflecting the symmetry of the configuration manifold, such laws not only exist but are moreover of great practical importance.

The third chapter is concerned with the quantization of the observables "multilinear in momentum", and in particular with the

delimitation of the possible operators of formal quantization as circumscribed by the requirement of (operator) symmetry, and the question of the essential self-adjointness of local observables associated with the multilinear momenta. Finally some possible means of determining an exact quantization are discussed and contrasted, and a tentative selection made of a particular scheme which is then illustrated by concrete example on the real line with the usual metric.

We conclude this preface with a brief indication of the layout of the thesis: Each chapter or associated group of appendices has been treated, for the purpose of all textual numbering and referencing systems, as a separate unit, and is prefixed by a detailed list of contents, and concluded by the appropriate group of references; so that all pointers of a chapter or group of appendices refer, unless otherwise indicated, to the text of that chapter or group of appendices. Finally note that a bibliography has been included which will serve as a collected list of references to papers and books employed.

K. McFarlane

Declarations

I declare this thesis to be of my own composition,
to be a record of my own work,
and not previously to have been presented in application for a higher
degree.

K. McFarlane

I declare that the conditions of the Resolution and the
Regulations appertaining to the degree of Doctor of Philosophy in
the University of St Andrews have been fulfilled.

K.K. Wan

Research Supervisor

Statement

I was admitted under Ordinance General No. 12 as a research student on the 1st of October 1976, and as a candidate for the degree of Doctor of Philosophy on the 1st of October 1977.

K. McFarlane

Chapter 1

"On the Quantization and Measurement of the Momenta"

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§1: Introduction.

The problem of the rigorous quantization of momentum observables (momenta) is of central importance to the understanding of quantum mechanics; for not only do momenta form the simplest class of observables, other than those functions without momentum dependence, but also their typical representatives, the linear and angular momenta, form the basis of the conservation laws of dynamics. It is clearly desirable that any proposed theory of their quantization should be formulated at a high level of abstraction, since only then can generality of application be anticipated. Viewed in this light, a Riemannian manifold M seems to be the natural medium of expression; for in the corresponding manifold-theoretic formalism the basic geometric entities constructed upon the manifold, as well as the manifold itself, have direct physical significance.

The basic work on the problem of the quantization of momenta is that of G.W. Mackey, in which it is demonstrated that to each complete momentum P (corresponding to a complete vector field over M), there exists a uniquely defined essentially self-adjoint operator $Q_0(P)$ over the natural Hilbert space $\mathcal{L}^2_p(M)$ of M , whose closure may be identified with the (unique) quantum observable $Q(P)$ analogous to P . This is an important and general result, which is nevertheless far from encompassing the quantization problem for the momenta. Such a total analysis requires the presence of each one of the following elements;

- [1] the explicit determination of the existing unique quantum observable corresponding to a complete momentum,
- [2] the discussion of the quantization of momenta which do not generate complete vector fields,
- [3] an analysis of the dequantization of quantum momenta, and

[4] the construction of a theory of measurement of the quantizable momenta, both in the classical and the quantum cases,

this last being necessary if the theoretical construction is to be comparable with experiment.

This chapter is the outcome of an attempt to construct such a self-contained general scheme of quantization by seeking to answer as far as possible the foregoing questions, and to explore the inter-relationships which obtain among them. Our analysis leads to a most pleasing conclusion, that the abstract and formal quantization condition of completeness prerequisite in Mackey's scheme does indeed have a direct physical foundation; for the quantizability condition on P may be traced to the concept of global measurability, introduced and discussed in the latter part of this chapter.

§2: The Quantization of Complete Momenta.

We adopt as our model of a quantum system that of Mackey^(1,2,3,4) in which the configuration space of the dynamical system is represented by a Riemannian manifold M of metric tensor G and corresponding density ρ , the phase space by the corresponding cotangent bundle T^*M , and the quantum mechanical Hilbert space by the set $L^2_\rho(M)$ of functions which are Lebesgue square-integrable with respect to the density ρ . This mathematical substructure provides a basis upon which both classical and quantum mechanics may be constructed. As to the representation of classical mechanics⁽⁵⁾, we need only note that to each classical momentum P , defined as a map¹ $P: T^*M \rightarrow \mathcal{R}$, there is associated a uniquely

¹ Explicitly⁽⁶⁾ $P(p,q) = p.X(q)$ results from the action of a one-form p on a vector field X of M , and in terms of a local chart (p_i, q^j) of T^*M we have $p = p_i dq^i$, $X = \xi^i \partial_i$ and $P = p.X(q) = p_i dq^i . (\xi^j \partial_j) = \xi^i p_i$.

defined vector field X on M . The explicit scheme of quantization proposed by Mackey comprises three elements:

- [5] The free Hamiltonian H has a quantum analogue $Q(H)$ which is postulated to be the Laplacian operator

$$Q(H) = -\frac{\hbar^2}{2m} \nabla^2, \quad (1)$$

on a domain of definition such that $Q(H)$ is self-adjoint.

- [6] The scalar functions $f: M \rightarrow \mathbb{R}$ are quantized in accordance with the rule

$$Q(f) = f, \quad (2)$$

on the domain,

$$DQ(f) = \{\psi \in \mathcal{L}^2_\rho(M) \mid Q(f)\psi \in \mathcal{L}^2_\rho(M)\}. \quad (3)$$

- [7] A prescription is provided for the quantization of a subclass of the classical momenta P , which are associated with complete vector fields X , and which we shall hereafter refer to as complete momenta. The identification of the quantum analogue $Q(P)$ of a complete momentum proceeds by several steps;

- (i) identification of the one-parameter-group of transformations of M , $\{\Phi_t \mid t \in \mathbb{R}\}$, provided by the flow Φ_t associated with the corresponding vector field X on M ,
- (ii) construction of the one-parameter-group of unitary transformations $\{U_t \mid t \in \mathbb{R}\}$ of $\mathcal{L}^2_\rho(M)$ naturally induced by $\{\Phi_t \mid t \in \mathbb{R}\}$,
- (iii) identification of the unique self-adjoint operator Ω such that $\forall t \in \mathbb{R} \quad U_t = \exp\left(\frac{i}{\hbar} \Omega t\right)$ with the quantum

counterpart $Q(P)$ of P , and finally

(iv) prescription of an essentially self-adjoint operator

$Q_0(P)$ whose closure may be identified with the quantum observable $Q(P)$.

We may state this last result explicitly in the following theorem which will serve as the starting point of our analysis.

Theorem 1: On the Quantization of Complete Momenta.

If P is a complete momentum observable over T^*M generating a C^∞ vector field X on M , then the symmetric operator $Q_0(P)$ defined by

$$Q_0(P) = -i\hbar(X + \frac{1}{2} \operatorname{div} X), \quad (4)$$

with domain,

$$DQ_0(P) = \{\psi \in L^2_\rho(M) \mid \psi \in C^\infty_0(M), Q_0(P)\psi \in L^2_\rho(M)\}, \quad (5)$$

where $\operatorname{div} X$ denotes the divergence² of the vector field X , and where $C^\infty_0(M)$ denotes the set of infinitely differentiable functions of compact support, is essentially self-adjoint, and hence possesses a unique self-adjoint extension which is identified with the quantum observable $Q(P)$.

Proof: see appendix 1, Mackey⁽⁸⁾, Varadarajan⁽⁹⁾, Hermann⁽¹⁰⁾, Abraham and Marsden⁽¹¹⁾.

² The divergence has the implicit manifold-theoretical definition,

$$\operatorname{div} \langle X, \rho \rangle = \operatorname{div} X \cdot \rho$$

where

$$\operatorname{div} \langle X, \rho \rangle = \lim_{t \rightarrow 0} \frac{\Phi_t^* \rho - \rho}{t},$$

the notation being that of Loomis and Sternberg⁽⁷⁾.

It has, moreover, proved possible to give the explicit expression of the operator $Q(P)$, a generalization of the work on one-dimensional manifolds of Wan and Viazminsky⁽¹²⁾.

Theorem 2: The Explicit Representation of a Complete Quantum Momentum.

The quantum analogue $Q(P)$ of a complete momentum P as introduced in the previous theorem is given explicitly by

$$Q(P) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) , \quad (6)$$

with domain,

$$DQ(P) = \{\psi \in \mathcal{L}^2_\rho(M) \mid \psi \in C^1(X, M), Q(P)\psi \in \mathcal{L}^2_\rho(M)\} , \quad (7)$$

where D_X is the Lie derivative operation (with respect to X), and where $C^1(X, M)$ is the set of functions on M whose Lie derivative with respect to X exists.

Proof: see appendix 2.

The nature of the action of (6) and of the domain (7) may be in some detail illustrated by means of a coordinate-based interpretation. Letting $\{x^i \mid i \in [1, n]\}$ denote³ a coordinate system in some local chart U of M in terms of which

$$X = \xi^i \frac{\partial}{\partial x^i}, \quad G = g_{ij}(x^k), \quad \rho = \sqrt{g} = (|\det g_{ij}|)^{\frac{1}{2}}, \quad (8)$$

we note:

[8] If $\psi \in C^1(M)$ is a once-differentiable function on M , then

$\psi \in C^1(X, M)$ and $D_X \psi = X\psi$, so that (6) becomes simply

$$Q(P)\psi = -i\hbar(X + \frac{1}{2} \operatorname{div} X)\psi , \quad (9)$$

³ The set $[1, n]$ is a shorthand for $\{1, 2, 3, \dots, n\} \subset \mathbb{N}$.

and, in the local chart U , has the representation,

$$Q(P)\psi = -i\hbar\left(\xi^i \frac{\partial}{\partial x^i} + \frac{1}{2\sqrt{g}} \frac{\partial}{\partial x^i} (\xi^i \sqrt{g})\right)\psi. \quad (10)$$

However, since $\psi \in C^1(X, M)$ does not imply that $\psi \in C^1(M)$, it is misleading in our present context to write,

$$D_X = X = \xi^i \frac{\partial}{\partial x^i}; \quad (11)$$

for the right-hand expressions imply, albeit implicitly, a domain of operation consisting of functions which are once-differentiable with respect to every coordinate x^i , $i \in [1, n]$.

- [9] In a coordinate chart V of coordinatization $\{\bar{x}^i | i \in [1, n]\}$ in which X assumes the canonical form $\frac{\partial}{\partial \bar{x}^1}$ we have that $\psi \in DQ(P)$ implies that ψ is once differentiable with respect to \bar{x}^1 and, therefore, that

$$Q(P)\psi = -i\hbar\left(\frac{\partial}{\partial \bar{x}^1} + \frac{1}{2\sqrt{g}} \frac{\partial}{\partial \bar{x}^1} (\sqrt{g})\right), \quad (12)$$

in an obvious notation. Such a chart, which we may term canonical, may be constructed to contain any point of M at which $X \neq 0$. (13)

- [10] At critical points where by definition $X = 0$ we have that

$$D_X = 0, \text{ div } X \neq 0,^4 \text{ and } Q(P) = -\frac{1}{2}i\hbar \text{ div } X, \quad (13)$$

⁴ Note that, whereas $X(x) = 0 \not\Rightarrow (\text{div } X)(x) = 0$, it is nevertheless true that, if the set $K = \{x \in M | X = 0\}$ is of non-zero measure, then the symmetry of $Q_0(P)$ implies (cf appendix 2) that $\text{div } X = 0$ almost everywhere in K ; so that, regarding $\text{div } X$ as a Hilbert space function in $\mathcal{L}^2_\rho(M)$, we may equivalently take $\text{div } X = 0$ whenever $X = 0$, when (13) assumes the simpler form $Q(P) = 0$.

which simply states that at isolated critical points, or over extended critical sets, the functions $\psi \in DQ(P)$ need not be differentiable at all.

We may exemplify in their turn these remarks by considering the case of the Euclidean plane, \mathbb{R}^2 with the usual metric, upon which is defined the classical angular momentum observable L_z . In terms of global Cartesian coordinates (x, y) of \mathbb{R}^2 and the corresponding chart (x, y, p_x, p_y) of $T^*\mathbb{R}^2$, L_z has the familiar representation

$$L_z = xp_y - yp_x, \quad (14)$$

is associated with a C^∞ complete vector field X on \mathbb{R}^2 given by

$$X = x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}, \quad (15)$$

and has as quantum counterpart the self-adjoint operator over $L^2(\mathbb{R}^2)$,

$$Q(L_z) = -i\hbar D_X, \quad (16)$$

in which D_X acts upon its maximal domain as prescribed in (7).

If now $\psi \in C^1(\mathbb{R}^2)$ then clearly $Q(L_z)\psi = -i\hbar(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x})\psi$, so that, provided the later operator is assumed to have its conventional domain of $C^1(\mathbb{R}^2)$, we have

$$Q(L_z) \supset -i\hbar(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}). \quad (17)$$

It is nevertheless, as is tempting and is widely used in practice, incorrect to assert that the component expressions of (17) are equal, since the domain $DQ(L_z)$ contains functions which are differentiable with respect neither to x nor to y . In fact the true equality of which the commonly used device is a specialization is simply

$$Q(L_z) = \overline{-i\hbar(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x})}, \quad (18)$$

where the bar denotes the operation of closure, as may readily be seen

by noting that $Q_0(L_Z) \subset -i\hbar(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}) \subset Q(L_Z)$ and that $Q_0(L_Z)$ is essentially self-adjoint. The most general coordinate-based representation of $Q(L_Z)$ may be obtained at every point, else the origin, of \mathbb{R}^2 in terms of a local canonical chart in which the azimuthal angle θ about the origin relative to some fixed radius as base line plays the role of \bar{x}^1 of [9] above. At all points of such a local canonical chart, which may be extended to cover \mathbb{R}^2 almost everywhere, and for all states ψ in the domain of $Q(L_Z)$, we have that

$$Q(L_Z)\psi = -i\hbar \frac{\partial \psi}{\partial \theta}. \quad (19)$$

At the origin, at which the vector field X has a critical point, no state function in $DQ(L_Z)$ need be differentiable with respect to any coordinate variable.

Theorems 1 and 2 provide us with a (partial) scheme of quantization, applicable to complete momenta, which we shall argue is exhaustive in that all "quantizable" momenta are complete. We first establish the following result which is of central importance.

Theorem 3: On the Dequantization of a Quantum Momentum.

Let Ω be a self-adjoint operator on the Hilbert space $\mathcal{L}^2_\rho(M)$ possessing an essentially self-adjoint restriction Ω_0 defined by

$$\Omega_0 = -i\hbar(X + \frac{1}{2} \operatorname{div} X), \quad (20)$$

with domain,

$$D\Omega_0 = \{\psi \in \mathcal{L}^2_\rho(M) \mid \psi \in C^\infty_0(M), \Omega_0\psi \in \mathcal{L}^2_\rho(M)\}; \quad (21)$$

then the C^∞ vector field X generated by Ω_0 , and the corresponding classical momentum P are complete, (except perhaps on a set of measure zero^{5, 6}).

Proof: see appendix 3, Abraham and Marsden⁽¹⁴⁾.

It is now immediate that, discounting the qualification⁶ on completeness in theorem 3, we may introduce a bijective mapping between Π_C , the set of all complete C^∞ classical momenta over M , and Ω_C , the set of all self-adjoint operators as defined in theorem 3, given by the operations of quantization $Q: \Pi_C \rightarrow \Omega_C$, and of dequantization $Q^{-1}: \Omega_C \rightarrow \Pi_C$; so that the operation of quantization can give rise to difficulty only for incomplete momenta, (momenta associated with incomplete vector fields). It is this case which we now proceed to discuss.

§3: The Quantization of Incomplete Momenta.

The question now arises: what are the quantum analogues of the incomplete momenta? Clearly for an incomplete momentum P , $Q_0(P)$ cannot be essentially self-adjoint; hence either

- [11] $Q_0(P)$ has no self-adjoint extensions, which we interpret as meaning that no quantum observable $Q(P)$ associated with P exists, or else

⁵ This phrase is to be taken as meaning that all the maximal integral curves of X , except possibly those originating from a set of measure zero, are complete; or symbolically that,

$$\mu(A) = \int_A \rho = 0, \text{ where } A = \{x \in M \mid \{t \in \mathbb{R} \mid \Phi_t(x) \in M\} \neq \mathbb{R}\}.$$

⁶ This qualification, which does not seem to have relevance in the physical arguments of the sequel, may be regarded as arising from "irregularity" in the manifold rather than in the momentum; for example the C^∞ vector field $X = \frac{\partial}{\partial x}$ is complete on \mathbb{R}^2 , but complete except on a set of measure zero on $\mathbb{R}^2 - \{0\}$. In addition observe that

- (i) the distinction between completeness and completeness except on a set of zero measure does not appear in one-dimensional manifolds; and that
- (ii) the word "complete" may alternatively be taken to mean complete except on a set of measure zero, when the statements above regarding the operation of quantization are strictly correct.

[12] $Q_0(P)$ has many self-adjoint extensions, when the problem reduces to whether any, and if so which, extension is the quantum analogue $Q(P)$ of P .

We may shed light on the discussion of subclass [12] above by considering an example, which we take to be the linear momentum observable on a modified infinite square-well, and which we model on the manifold $M = (-1,1)$ with the metric tensor $G = g = (1-x^2)^{-2}$ and corresponding density $\rho = \sqrt{g} = (1-x^2)^{-1}$. The choice of the metric g is motivated by the following consideration; that, unless the well-width $\int_{-1}^1 \sqrt{g} dx$ is infinite, then neither

[13] will the symmetric operator $Q_0(H)$ generated by the free classical Hamiltonian H and given by

$$Q_0(H) = -\frac{\hbar^2}{2m} (1-x^2) \frac{d}{dx} (1-x^2) \frac{d}{dx}, \quad (22)$$

on the domain,

$$DQ_0(H) = \{\psi \in L^2_{\sqrt{g}}(-1,1) \mid \psi \in C_0^\infty(-1,1), Q_0(H)\psi \in L^2_{\sqrt{g}}(-1,1)\}, \quad (23)$$

be essentially self-adjoint, so that there will exist⁷ no unique self-adjoint Laplacian which may be identified with the free quantum Hamiltonian $Q(H)$, nor

[14] will the Riemannian space (M,G) be geodetically complete, so that a classical particle cannot execute free motion along the geodesics of M without at some time suffering abrupt discontinuities in its momentum upon "reflection from the walls of the well".

⁷This remark is demonstrated in theorem 4.

Our chosen model system, avoiding both of the difficulties [13] and [14], possesses a unique well-defined free quantum Hamiltonian $Q(H)$.

The linear momentum P , corresponding to the incomplete vector field $\frac{d}{dx}$ on $(-1,1)$, has as quantum analogue a self-adjoint extension of $Q_0(P)$ given by

$$Q_\beta(P) = -i\hbar\left(\frac{d}{dx} + \frac{x}{1-x^2}\right), \quad (24)$$

with domain,

$$\begin{aligned} DQ_\beta(P) = \{ \psi \in \mathcal{L}^2_{\sqrt{g}}(-1,1) \mid \psi \in C^1(-1,1), Q_\beta(P)\psi \in \mathcal{L}^2_{\sqrt{g}}(-1,1), \\ \lim_{x \rightarrow -1} (1-x^2)^{-\frac{1}{2}}\psi = \lim_{x \rightarrow +1} (1-x^2)^{-\frac{1}{2}}\psi e^{i\beta} \}, \end{aligned} \quad (25)$$

where $\beta \in [0, 2\pi)$ is any fixed number.

The spectrum of $Q_\beta(P)$ is discrete and the "levels" non-degenerate of eigenfunctions,

$$\psi_n^\beta(x) = [\tfrac{1}{2}(1-x^2)]^{\frac{1}{2}} \exp(-i \frac{p_n}{\hbar} x), \quad n \in \mathbb{Z}, \quad (26)$$

and eigenvalues,

$$p_n = p_0 + n\pi\hbar, \quad p_0 = \tfrac{1}{2}\beta\hbar, \quad n \in \mathbb{Z}. \quad (27)$$

This completes the specification of the system.

Consider now the performance of the following sequence of measurements;

[15] perform a measurement of $Q_\beta(P)$ on the system and thus

prepare the system in some eigenstate ψ_n^β ;

[16] measure $Q_\gamma(P)$, $\gamma \neq \beta$, on the system.

Then, since $\psi_n^\beta \notin DQ_\gamma(P)$, it follows that $\langle \psi_n^\beta | Q_\gamma(P) | \psi_n^\beta \rangle$ is undefined, so that physically the result of the above sequence of measurements is an infinite average value of $Q_\gamma(P)$, and the assumption underlying the

procedure, that $Q_\beta(P)$ and $Q_Y(P)$ are both observables corresponding to attributes of the system, gives rise to an inconsistency. Hence at most one of the $Q_\beta(P)$ can be a system observable, which lends support to the thesis, embodied in subclassification [12] above, that the operation of quantization is a bijective mapping whose inverse is the dequantization operation.

The situation is still serious, however, even if we admit that a particular $Q_\beta(P)$ is the true quantum analogue of P (which assumption is very difficult to justify) since there would seem to be no a priori valid criterion to decide among the various $\beta \in [0, 2\pi)$. In this context it has been suggested by Capri⁽¹⁵⁾ that, in the case of the usual (unmodified) infinite square-well, auxiliary conditions upon the admissible states, such as $\psi(1) = \pm\psi(-1)$, may be imposed on physical grounds as being part of the specification of the problem. These constraints cannot, however, be absorbed into a formalism which employs only the concepts of configuration manifold and density, ($M = (-1, 1)$, $\sqrt{g} = 1$, say), since the corresponding Hilbert space necessarily contains vectors which violate any such boundary constraint. In particular it is clear that, independent of the knowledge of any such boundary condition which appertains to a particular physical system, no unique $Q_\beta(P)$ can be chosen a priori, since each possible boundary condition of the form $\psi(1) = e^{i\beta}\psi(-1)$ results in a distinct operator $Q_\beta(P)$, and in a different physical interpretation of the model system.

Nor, moreover, is it possible to determine $Q_\beta(P)$ by recourse to experiment, since if an apparatus may be constructed to measure $Q(P) = Q_{\beta_0}(P)$, then the resultant discrete spectrum of values can be arbitrarily well approximated by some $Q_\beta(P)$, $\beta \neq \beta_0$, and hence the (inexact) experimental spectrum cannot be used to determine $Q(P)$ a posteriori.

As a final observation we note that, if the condition that $Q_0(H)$ be essentially self-adjoint is relaxed, thus regaining the symmetry

between the two forms H and P , then, since in general $\psi_n^\beta(P) \notin DQ(H)$ $\forall \beta \in [0, 2\pi)$, where $Q(H)$ denotes the usually preferred⁽¹⁶⁾ free quantum Hamiltonian of the (unmodified) infinite square-well, the inconsistency is again apparent, and the model untenable.

Thus the analysis of this section will be seen to have identified some of the difficulties which arise from an attempt to quantize incomplete momenta; in the sequel we shall examine this problem from a radically different standpoint by developing a theory of the measurement of both classical and quantum mechanical observables, an analysis which will lead to striking insight into the physical origins of the problem. Before proceeding to so do, however, we pause in our development to discuss in some detail the theory of the Hamiltonian and the momenta in a one-dimensional manifold.

54: A detailed study of the Complete Momenta and Hamiltonians on the infinite Square-Well.

We now proceed to examine in detail the complete momenta and Hamiltonians on the manifold $M = (a, b)$, $a, b \in \mathbb{R}$, with a view to giving a comprehensive analysis of the infinite square-well model, since in this case it is possible to specify in considerable detail the nature of the actual quantum operators.

We begin with the classical free Hamiltonian, $H = \frac{1}{2m} g^{-1} p^2$, of the system and give a criterion that $Q(H)$ shall be uniquely determined, or equivalently that $Q_0(H)$ shall be essentially self-adjoint. This is embodied in the following theorem.

Theorem 4: A criterion for the "completeness" of the Hamiltonian.

Let \sqrt{g} be the C^∞ density on a Riemannian manifold $(a, b) \subset \mathbb{R}$, and let $Q_0(H)$, the symmetric operator prescribed⁸ by the classical free Hamiltonian be

$$Q_0(H) = -\frac{\hbar^2}{2m} \nabla^2 = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{d}{dx} \frac{1}{\sqrt{g}} \frac{d}{dx}, \quad (28)$$

on the domain,

$$DQ_0(H) = \{\psi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \mid \psi \in C_0^\infty(a,b), Q_0(H)\psi \in \mathcal{L}^2_{\sqrt{g}}(a,b)\}. \quad (29)$$

Then $Q_0(H)$ is essentially self-adjoint if and only if the Riemannian space (M, \sqrt{g}) has complete geodesics, or equivalently is geodetically complete.

Proof: see appendix 4.

We may, moreover, give $Q(H)$ arising from an essentially self-adjoint $Q_0(H)$ explicitly, and specify the spectral operator and corresponding spectrum, which results comprise the following theorem.

Theorem 5: On the free quantum Hamiltonians.

The quantum analogue $Q(H)$ of the classical free Hamiltonian $H = \frac{1}{2m} g^{-1} p^2$, on the geodetically complete Riemannian space $\{(a,b), \sqrt{g}\}$, is given by

$$Q(H) = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{d}{dx} \frac{1}{\sqrt{g}} \frac{d}{dx}, \quad (30)$$

with domain,

$$DQ(H) = \{\psi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \mid \psi \in C^2(a,b), Q(H)\psi \in \mathcal{L}^2_{\sqrt{g}}(a,b)\}, \quad (31)$$

and may be written as

$$Q(H) = \frac{1}{2m} Q^2(P), \quad (32)$$

where P is the complete momentum $\frac{1}{\sqrt{g}} p$.

Proof: see appendix 4.

⁸ The choice of the Laplacian operator in the differential expression of $Q_0(H)$ is axiomatic in Mackey's scheme, but can be justified by requiring that $Q_0(H)$ commute with all the "motions", or rather their unique quantum analogues, of a space of constant curvature, of which (\mathbb{R}^n, \sqrt{g}) is an example. See Han and Viazminsky⁽¹⁷⁾ for details.

These theorems⁹ exhaust the description of the free quantum Hamiltonians, which we observe by theorem 4 exist only in spaces which are (metrically) unbounded, so that any $x_0 \in (a,b)$ is infinitely remote in real distance from the "boundaries" $x = a$, and $x = b$, of the manifold. In consequence a classical free particle, following a geodetic path, never encounters the system boundary and hence experiences neither "reflection" nor any other discontinuous disturbances of its motion which must otherwise occur. This clearly shows that difficulties arise even for the classical motion in spaces in which $Q_0(H)$ is not essentially self-adjoint.

The exposition for the complete momenta is parallel to that for the Hamiltonians. We first give a criterion that $Q_0(P)$ be essentially self-adjoint, or equivalently that the momentum P be complete.

Theorem 6: A criterion for the completeness of a momentum.

Let \sqrt{g} be the C^∞ density on the Riemannian manifold (a,b) , and let $P = \xi(x)p$ be a momentum corresponding to a vector field $X = \xi(x) \frac{d}{dx}$, where $\xi(x)$ is C^∞ on the closed interval $[a,b]$. Then P is complete if and only if $\xi(a) = \xi(b) = 0$.

Proof: see appendix 5.

We note that this result is, as anticipated, independent of the metric \sqrt{g} , and, being so simple, is of great convenience and utility. There remains only the specification of the unique $Q(P)$ generated by a complete momentum P and to give explicitly the corresponding spectral operator and spectrum. Again we state the result as a theorem.

Theorem 7: On the complete quantum momenta.

The quantum analogue $Q(P)$ of a complete momentum $P = \xi(x)p$ defined over a manifold $M = (a,b)$ of C^∞ density \sqrt{g} , and

⁹ The above theorem 6 and subsequent text justify and amplify upon the remarks [13]-[14] made concerning $Q(H)$ in the preceeding §3.

generating a C^∞ vector field $X = \xi(x) \frac{d}{dx}$, is given¹⁰ by

$$Q(P) = -i\hbar\left(\xi \frac{d}{dx} + \frac{1}{2\sqrt{g}} \frac{d}{dx} (\xi\sqrt{g})\right), \quad (33)$$

with domain,

$$DQ(P) = \{\psi \in L^2\sqrt{g}(a,b) \mid \psi \in C^1(X,M), Q(P)\psi \in L^2\sqrt{g}(a,b)\}. \quad (34)$$

Further there exists a partition, $\{K_n \mid n \in \mathbb{N} \setminus \{0\}\}$, of M , (furnished by K_0 , the set of critical points of X , and $\{K_n \mid n \in \mathbb{N}\}$, the partition of $M - K_0$ into maximal connected subsets), in terms of which the spectral function $E(\lambda)$ of $Q(P)$ may be constructed.

The spectrum of $Q(P)$ is \mathcal{R} and $E(\lambda)$ is explicitly

$$E(\lambda) = \sum_{n \in \mathbb{N}} \chi(K_n) E(K_n, \lambda), \quad (35)$$

in which $\chi(K_n)$ is the characteristic function of K_n ,

$$E(K_0, \lambda) = H(\lambda), \quad (36)$$

is the Heavyside unit-step function⁽¹⁸⁾,

$$E(K_n, \lambda) \phi = \int_{-\infty}^{\lambda} \psi(K_n, \lambda) \int_{K_n} \phi \psi^*(K_n, \lambda) \sqrt{g} \, dx \, d\lambda, \quad (37)$$

and $\psi(K_n, \lambda)$ is the "localized eigenfunction" in K_n ,

$$\psi(K_n, \lambda) = (2\pi\xi\sqrt{g})^{-\frac{1}{2}} \exp(i\lambda/\hbar \int_{x_0}^x \xi^{-1} dx), \quad x_0, x \in K_n. \quad (38)$$

Proof: see appendix 5.

¹⁰ The differential expression (33) is correct everywhere on M provided that the symbol $\xi \frac{d}{dx}$ is regarded as being by definition zero whenever $\xi(x) = 0$.

For the special case of a complete momentum "without critical points" the spectral function $E(\lambda)$ is greatly simplified, and is given by the following theorem.

Theorem 8: On the spectral operator of a complete momentum without critical points.

Let $Q(P)$ be the quantum analogue of a momentum $P = \xi(x)p$ generating a complete C^∞ vector field $X = \xi(x) \frac{d}{dx}$ without critical points on $\{(a,b), \sqrt{g}\}$. Then $Q(P)$ has a spectral function $E(\lambda)$ given by

$$E(\lambda)\phi = \int_{-\infty}^{\lambda} \psi(\lambda, x) \int_a^b \phi\psi^*(\lambda, x)\sqrt{g} \, dx \, d\lambda, \quad (39)$$

in which $\psi(x, \lambda)$ is the generalized eigenfunction,

$$\psi(x, \lambda) = (2\pi\xi\sqrt{g})^{-\frac{1}{2}} \exp(i\lambda/\hbar \int_{x_0}^x \xi^{-1} dx), \quad x_0, x \in (a, b). \quad (40)$$

Proof: corollary to theorem 7.

This completes our discussion of the infinite square-well.

§5: The Classical Measurement of Momenta.

The goal of this section is to construct the concept of classical global measurability and to relate it to the completeness of a momentum. The analysis is structured as follows: having first motivated the discussion of the proposed model of classical measurement based upon an impulsive collision between test and reference particle by a discussion of the measurement of Cartesian momenta on a Euclidean space, we proceed first to develop the theory of the collisional process in a general Riemannian space, and then to discuss its local application in the determination of the momentum P associated with a given test particle. Finally the ideas developed in the analysis of

local measurements are combined to afford the concept of global measurability and the link with completeness is established.

§5.1: Classical momentum measurement in Euclidean space.

Consider initially the simplest case of the measurement of the linear momentum of a free particle moving in one-dimension, which we model on the configuration manifold $M = \mathbb{R}$ with the usual metric by the momentum p conjugate to the global Cartesian coordinate y . A measurement of p necessarily involves a non-zero, though perhaps very small, displacement of the measured particle, as is sufficiently clear from the very definition of p , namely $p = \lim_{\epsilon \rightarrow 0} (y(t+\epsilon) - y(t))/\epsilon$, where $y(t)$ is the particle trajectory as a function of time; for if the particle is allowed no recoil during measurement, then for all sufficiently small ϵ we have that $y(t+\epsilon) = y(t)$, and thus that $p = 0$, which is clearly absurd. This recoil property is embodied in the impulsive measurement model of Aharanov and Safko⁽¹⁹⁾, of which the following is an example¹¹.

We elect to measure the momentum of the above test particle by measuring the recoil displacement of a second particle of momentum \bar{p} , conjugate to the position coordinate \bar{y} , with which it interacts in accordance with the Hamiltonian,

$$H = p^2/2m + \bar{p}^2/2\bar{m} + \omega(t)p\bar{p}, \quad (41)$$

in which $\omega(t)$ is the function prescribing the interaction and is given by

$$\omega(t) = \begin{cases} \omega_0 & t \in (0, \tau) \\ 0 & t \notin (0, \tau) \end{cases}. \quad (42)$$

The equations of motion of the test and measuring particles are therefore

¹¹Whereas Aharanov and Safko consider quantum measurements, we modify the model to discuss classical ones.

$$\begin{aligned} y(t) - y(o) &= pt/m + \omega t \bar{p}, \\ \bar{y}(t) - \bar{y}(o) &= \bar{p}t/\bar{m} + \omega t p. \end{aligned} \quad (43)$$

Taking the impulsive limit, $\tau \rightarrow 0$, of an instantaneous contact interaction, such that $\omega_0 \tau = \sigma$ remains finite (for otherwise the interaction has no perceptible effect) we deduce

$$\begin{aligned} \Delta y &= y(\tau) - y(o) = \sigma \bar{p}, \\ \Delta \bar{y} &= \bar{y}(\tau) - \bar{y}(o) = \sigma p. \end{aligned} \quad (44)$$

Thus we see that, if the value of σ characteristic of the interaction is known, then p is measurable in terms of the displacement (recoil) $\Delta \bar{y}$ of the reference particle. We note particularly that only the recoil $\Delta \bar{y}$ is required, so that the exact absolute position of the particle under test need not be known, provided only that the recoil is measurable. This analysis shows that, at least in this particular example, the momentum p may be measured by this procedure, wherever the particle lies in the configuration manifold, in a manner independent of, and without knowledge of, position.

The situation is radically different if we choose as configuration manifold a proper subset of \mathcal{R} , so that the momentum p , and the geodesics of the Riemannian space, are incomplete; for the above analysis cannot fully be carried out. The problem first arises with the equations of motion (43), which are valid only if $y(t)$, and $\bar{y}(t)$ lie in M , conditions not generally satisfied for times $t > 0$, and which therefore give rise to position dependent constraints. Consequently the procedure of taking the impulsive limit can be carried out only if $y(\tau), \bar{y}(\tau) \in M$, or equivalently

$$y(o) + \Delta y = \sigma \bar{p} + y(o) \in M, \quad \bar{y}(o) + \Delta \bar{y} = \sigma p + \bar{y}(o) \in M. \quad (45)$$

These equations serve to define a subregion of the manifold, determined by the momentum p and the collisional parameter σ within which a

momentum determination, using such a collision as a measuring device, is possible. It is clear, moreover, that for any fixed σ a value of p may be chosen such that $|\Delta \bar{y}|$ exceeds any preassignable limit; so that not only is for a fixed momentum value p the range of points at which p is measurable a proper subset of the manifold, but also no point of M will admit a measurement of an arbitrarily large p -value for a fixed value of σ . Thus a momentum may not, in general, be measured by an impulsive collision of fixed characteristic parameter σ , wherever the corresponding particle lies in the manifold.

A similar situation obtains between \mathcal{R}^n and its proper subsets, where the components of the linear (Cartesian) momentum p_i are conjugate to global Cartesian coordinates $\{y^i | i \in [1, n]\}$. The interaction Hamiltonian is simply

$$H = \frac{1}{2m} \delta^{ij} p_i p_j + \frac{1}{2\bar{m}} \delta^{ij} \bar{p}_i \bar{p}_j + \omega(t) \delta^{ij} p_i \bar{p}_j, \quad (46)$$

where δ^{ij} is Kronecker delta, and the recoil displacements of the colliding particles are related to their momentum values by

$$\begin{aligned} \Delta y^i &= \sigma \bar{p}_i, & y^i(o) + \Delta y^i &\in M, \\ \Delta \bar{y}^i &= \sigma p_i, & \bar{y}^i(o) + \Delta \bar{y}^i &\in M. \end{aligned} \quad (47)$$

Hence we have demonstrated that, even in the simplest possible case of the linear momentum defined upon a set of \mathcal{R} with the usual metric, there arises, with regard to their measurability by a pre-elected collisional process, a fundamental distinction between complete momenta on spaces with complete geodesics, and incomplete momenta on spaces with incomplete geodesics. We shall proceed, therefore, to investigate this distinction in the more general context of a momentum defined upon a Riemannian manifold, our first task being to develop an equation analogous to (44) describing in the general case the relationship between the measured recoil and the corresponding momentum value.

§5.2: Classical momentum measurement in Riemannian space.

The problem herein lies in the measurement of a momentum P , generating a corresponding vector field X without critical points¹², on a Riemannian manifold M of metric G . At every point $x \in M$ there exists a local chart¹³ of coordinatization $\{x^i | i \in [1, n]\}$ in which X assumes the canonical form $\frac{\partial}{\partial x^1}$. In this chart the momentum P has coordinate representation p_1 , conjugate to x^1 , and the metric G assumes the tensor form $g^{ij}(x^k)$. The model measuring system is a collision between two particles; one the test particle described by unbarred coordinates; the other the reference (measuring) particle described by barred coordinates; the measured parameter is the reference particle recoil. As the Hamiltonian describing the collision we elect the natural extension of (41) and (46), namely

$$H = \frac{1}{2m} g^{ij} p_i p_j + \frac{1}{2\bar{m}} g^{ij} \bar{p}_i \bar{p}_j + \omega(t) \bar{g}^{ij} p_i \bar{p}_j, \quad (48)$$

in which $\bar{g}^{ij}(x^k, \bar{x}^l)$ is the parallel propagator¹⁴ generated by the metric $g^{ij}(x^k)$, and $\omega(t)$ is the interaction function (42).

The solution of Hamilton's equations of motion generated by (48) would, in general, prove a formidable task. Fortunately, however, it is sufficient for our purposes to determine the local motion in the neighbourhood of the collision, which is most simply given in terms of the local Cartesian coordinates, $\{y^i | i \in [1, n]\}$, about some neighbouring fixed point $x_0 \in M$. The equations of transformation connecting the coordinate systems are (Synge and Schild⁽²²⁾)

¹² We defer the discussion of the critical points until §7.

¹³ The transformation $\xi^i \frac{\partial}{\partial \bar{x}^i} \rightarrow \frac{\partial}{\partial x^1}$ is achievable at all points (x^i) of M for which $\xi^i(\bar{x}^k) \neq 0$, as is demonstrated in Eisenhart⁽²⁰⁾.

¹⁴ The parallel propagator is as defined in Synge⁽²¹⁾, though it should be noted that where many geodesics connect two points, the propagator is here defined in terms of one of least length. Note that, for sufficiently close, as here, points (y^i) , (\bar{y}^i) of the local Cartesian chart, the connecting minimal geodesic lying within that chart is unique.

$$y^i = b_j^i (x^j - a^j) , \quad (49)$$

where b_j^i is a matrix of constants, and the point x_0 has coordinate representation $(x^j) = (a^j)$. It is, moreover, possible, as is demonstrated in appendix 6, to elect b_j^i such that

$$y^1 = b_1^1 (x^1 - a^1) ; \quad (50)$$

so that, in terms of these coordinates the Hamiltonian (48) becomes¹⁵ simply

$$H = \frac{1}{2m} \delta^{ij} p_i^o p_j^o + \frac{1}{2m} \delta^{ij} p_i^{o-o} p_j^{o-o} + \omega(t) \delta^{ij} p_i^{o-o} p_j^{o-o} , \quad (51)$$

in which p_i^o is the (local) momentum conjugate to the coordinate y^i . The equations of transformation (50) yield (appendix 6) that $p_1 = b_1^1 p_1^o$, and Hamilton's equations of motion yield by (51), that $\sigma p_k^o = \Delta y^k$, $\sigma p_k^{o-o} = \Delta y^k$, whence we may deduce the equation connecting p_1 , the test particle's momentum, and Δy^1 , the measured (physical) displacement along y^1 , as simply

$$p_1 = \sigma^{-1} (b_1^1)^2 \Delta x^1 = \sigma^{-1} b_1^1 (x_0) \Delta y^1 , \quad (52)$$

all the other coordinate displacements being determined in terms of the test particle's (linear) momentum components by $\sigma p_k^o = \Delta y^k$; so that the reference particle recoils by an amount and in a direction determined by the test particle's momentum. Finally we note that it is always possible to arrange the orientation of the reference particle prior to the interaction such that $\bar{p}_i^o = 0$, $i \neq 1$, resulting in the recoil Δy^1 of the test particle lying along the principal (y^1 -) axis, as is portrayed in figure 1. We shall always adopt this option when employing the measuring procedure in the sequel.

¹⁵ Subject to the constraints imposed in footnote 13, we have that \bar{g}^{ij} tends to δ^{ij} , since g^{ij} approaches δ^{ij} , in the limit of coincidence of the two points (y^i) , (\bar{y}^i) .

§5.3: On local Classical measurement.

We examine in this section the conditions that are necessary if the above defined procedure of measurement is to be applicable to a momentum P , using at every point of the configuration manifold a "local" apparatus. To this end it will be necessary to introduce the concept of local measurement; the intuitive motivation for which arises from the following consideration, that, whereas the configuration space (considered here as a physical space) is large, and indeed typically infinite, the "sensitive volume" of any local apparatus will not only be finite but also typically small. That is that global measurements can be obtained only by the combination of many (usually infinitely many) purely local measurements each conducted within a characteristic local set A .

Consider now the process of a local momentum measurement conducted within the finite local set A . We may abstract two features of the measuring procedure.

[17] No account is taken of position or momentum values out-with A ; so that if a (Cartesian or other) momentum is to be determined within A by means of the above impulsive collision then neither the test particle incident, nor the reference particle employed in the measurement, can so recoil as to leave the set A . Clearly this is simply a statement of the idea present in the term "sensitive volume".

[18] The set A must possess a least physical size; that is it must contain an open sphere S of some locally fixed radius $d_0 \neq 0$ "centred"¹⁶ upon some $x \in A$; so that, for a locally

¹⁶ By "centred" on $x \in A$ we mean precisely that the set $S = \{y \in M \mid d(x, y) = d_0\}$ is topologically equivalent to some S^n .

fixed range of particle energies $E \leq E_0$, such a local apparatus will be capable of recording the momentum P .

This requirement is necessary if, independent of a knowledge of the measured particle's direction of approach, the apparatus is to be capable of recording the Cartesian momenta p_i^0 of the incident particle and therefore of recording, via (52), any momentum P ; for otherwise it is possible to so allign an incident test particle of arbitrarily small kinetic energy $E \neq 0$, that the recoil $\sigma\sqrt{2mE}$ of the reference particle from its initial position at $x \in A$ will be of a sufficient magnitude as to cause the reference particle to leave A , so that by [17] the corresponding momentum value cannot be assigned.

In addition it is necessary that the local set A satisfy two further constraints, so that the analysis and in particular formula (52) of the previous section may be used to describe the impulsive measuring process within A . These conditions are

[19] that the set A is coverable by a local canonical chart $\{x^i | i \in [1, n]\}$ in terms of which the momentum P assumes the coordinatization p_1 conjugate to x^1 ,

and

[20] that the set A is sufficiently small that the departure within A of the manifold M from a Euclidean space is negligible.

Under these conditions the local Cartesian chart $\{y^i | i \in [1, n]\}$ of equations (49) and (50) is well defined within A , and the value of the momentum P is given, in a more elegant notation, by

$$P = b_1^1(x_0)P_0, \quad (53)$$

where $x_0 \in A$ is the origin, in the neighbourhood of the collision between test and measuring particles, of the local Cartesian system $\{y^i | i \in [1, n]\}$, and where $P_0 = p_1^0$, conjugate to y^1 , is the local (aligned) Cartesian momentum.

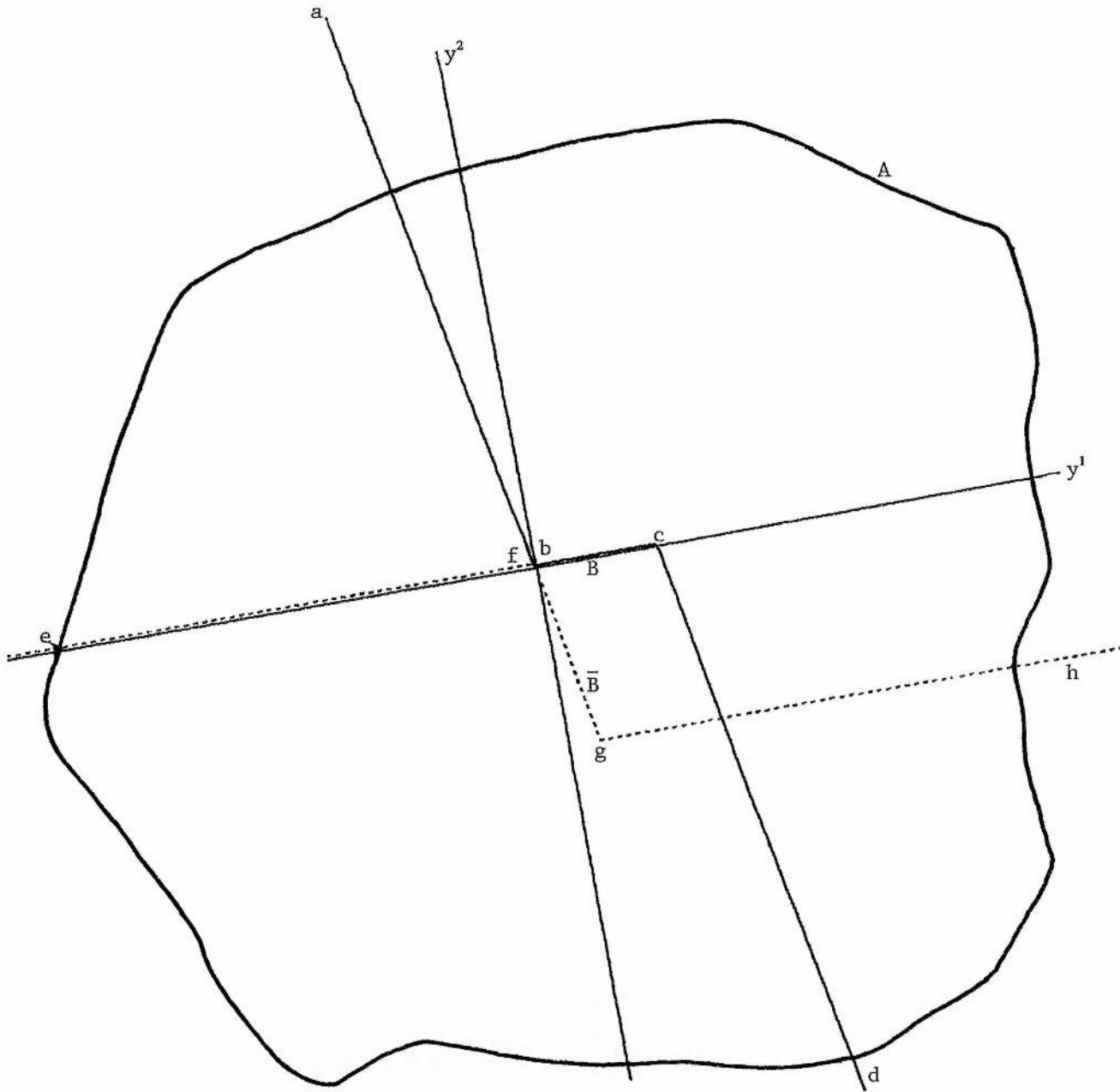
P_0 is itself determined in terms of the (metrical) recoil Δy^{-1} of the reference particle by

$$P_0 = \sigma^{-1} \Delta y^{-1}, \quad (54)$$

in which σ is the parameter marking the collision process and is assumed known.

There are, contained in the above measuring process, essentially only two distinct sources of possible error, that in the measurement of the reference particle recoil and therefore in the evaluation of the aligned local Cartesian momentum P_0 , and that in the identification of the point $x_0 \in A$ from which may be calculated P by (53). We shall assume that the former source of error may be made vanishingly small, or consequently that an arbitrarily accurate measurement may be made of P_0 , provided only that the recoil displacements Δy^{-i} lie within the local set A . The latter source of error, however, has an intrinsic physical significance arising from the impulsive nature of the collision between test and reference particles, which cannot be eliminated by perfection of the apparatus. This may be seen by a closer examination of the nature of the impulsive collision, the exact situation being as depicted in figure 1 overleaf. The test particle of momentum P recoils within the (one-dimensional) set B whose extent is determined solely by parameters intrinsic to the apparatus, the reference particle momentum \bar{p}_1^0 , and the collisional parameter σ ; and the reference particle recoils within a second (one-dimensional) set \bar{B} whose length and orientation are determined by the incident test particle. It is the finite (non-zero) extent of the set B intrinsic to the apparatus, and indeed to all

Figure 1: The geometry of the test/reference particle collision within the local set A.



The trajectory of the test particle of Cartesian momenta p_i^0 is the arc $abcd$, the local recoil set B demarking the extent of the uncertainty in position of the test particle during the collision; and the trajectory of the reference particle, aligned with the local flow direction efc and bearing Cartesian momentum \bar{p}_i^0 , is similarly $efgh$, the local set \bar{B} marking the recoil displacement of the reference particle during the collision.

classical measuring procedures, which gives rise to an irreducible error in the measurement of the momentum P ; for it is impossible to say at which point x of B the momentum P of the test particle was determined.

We are faced, therefore, with the problem of defining, (at least to some extent arbitrarily), the "value" attributed by an apparatus of sensitive volume A and recoil region B to the momentum P , and of quantifying the error which arises from the variability of $b_1^1(x)$ within B . To this end we propose the following description of a local measurement of P within A : In addition to the constraints [17]-[20] above, we impose upon the measuring procedure the following requirements;

[21] that the value of P_0 be determined exactly in the measurement,

[22] that the value attributed to the momentum P be calculated from the prescription,

$$P = b_1^1(B)P_0, \quad (55)$$

in which $b_1^1(B) = \int_B b_1^1(y^1) dy^1 / \int_B dy^1$ is the "mean" value of $b_1^1(y^1)$ within B , and

[23] that the error attributed to the measurement be given by

$$\Delta_B P = |P_0| \left(\int_B (b_1^1(y^1) - b_1^1(B))^2 dy^1 / \int_B dy^1 \right)^{\frac{1}{2}}, \quad (56)$$

or, equivalently, by the "standard deviation"⁽²³⁾ of $b_1^1(y^1)$ about its "mean" value in B .

The precise forms of (55) and (56) are based upon the following consideration, that the definitions of P and $\Delta_B P$ are compatible with a subjective probabilistic interpretation based upon the ignorance of

which particular $x \in B$ is the "correct" choice; for, if we assume that all points $x \in B$ are equally likely to be the choice from which to calculate P by (53) for a fixed value of P_0 , then we may identify $b_1^1(B)P_0$ with the least-squares estimator to P , and $\Delta_B P$ as the corresponding residual sum of squares⁽²⁴⁾. With this interpretation the terms "mean" and "standard deviation" above assume precise technical significance.

In summary we may observe that the two central features of a local measurement, the ability to record the momentum P of a particle to within a characteristic tolerance $\Delta_B P$, and the ability to do so for a given range of incident particle energies $E \leq E_0$, determine and are determined by the parameters which describe the dynamical process of the measurement, the reference particle momentum \bar{p}_1^0 , and the collisional parameter σ .

§5.4: Measurability and completeness.

It is now natural to enquire whether, and under what conditions, an apparatus of fixed sensitive volume may be employed at every point of the manifold M to measure a given momentum P to within a pre-assigned universally applicable tolerance Δ_0 . Such an apparatus, which we may term a standard apparatus, will be characterized by pre-assigned (non-zero) values of the dynamical parameters σ and \bar{p}_0^{-1} .

Consider firstly the conditions under which we may employ, universally within the configuration space M , such a standard apparatus to determine the local Cartesian momenta p_i^0 and hence the kinetic energies E of a class of incident test particles having a (globally) pre-assigned maximum energy E_0 . The ability to use such a standard apparatus centred on any particular $x \in M$ is, by [18] conditional upon there existing within the local sensitive volume $A \ni x$ an open ball of radius $d \geq \sigma\sqrt{2mE_0}$; so that the universal applicability of a standard

apparatus to measure a given range of energies is conditional upon the requirement that, around every $x \in M$, there exists, within the local set $A \ni x$, an open ball of (globally) fixed radius $d_0 = \sigma\sqrt{2mE_0}$. This analysis results immediately in the following theorem.

Theorem 9: Standard measurability and geodetic completeness.

It is possible to centre a standard apparatus of characteristic dimension $d_0 \neq 0$ at every point of the configuration manifold M only if¹⁷ M is geodetically complete.

Proof: see appendix 7.

This result is intuitively clear; for suppose that M is not geodetically complete, then it possesses a "boundary" and points may be chosen sufficiently close to this "boundary" that a region of radius d_0 cannot be constructed around them. It is important to observe that, if the space is not geodetically complete, then it is impossible, solely in terms of Hamilton's equations of motion derived from the Hamiltonian (51), to describe correctly the motions of test and reference particles during collisions sufficiently close to the spatial "boundaries" of the manifold, due to the presence of position-dependent constraints analogous to those discussed in §5.1. The measuring procedure is therefore intrinsically suspect when employed to measure any momentum P within a region sufficiently close to the "boundary" of M . Henceforth, therefore, we shall confine our attention exclusively to manifolds which are geodetically complete.

¹⁷ Observe that [20], which here assures [19], requires that within each local set A the departure from Euclidean space must be negligible. It may, in general, be impossible to assure this for the class of all sets of characteristic dimension $d_0 \neq 0$, regardless of how small d_0 is chosen.

We next consider, abstracting from our analysis of local measurement only the recoil sets B , the global behaviour of the characteristic errors $\Delta_B P$ which arise from an impulsive measurement of a momentum P , so as to introduce a concept of classical global measurability. The essential idea underlying this concept is that, for a suitably chosen reference class of local recoil sets B , the corresponding class of intrinsic uncertainties $\Delta_B P$ in the locally assigned values of the momentum P must be bounded above by some finite global tolerance or standard of accuracy Δ_0 . For, unless such a global standard $\Delta_0 \geq \Delta_B P$ exists, the accuracy of the local values of P decreases without limit as B is varied within its reference class; so that a fixedly reliable momentum value is not everywhere assignable, or, as we may say, P is not (classically) globally measurable. Turning our attention to more detailed considerations, we note that to be directly comparable with completeness the concept of classical global measurability must necessarily depend only upon properties of the momentum P or equivalently of the associated vector field X , so that the various local errors $\Delta_B P$ within an elected reference class must first be standardized to eliminate dependence upon the properties of the particles under test. This is readily achieved by requiring

[24] that the aligned Cartesian momentum be taken in the calculation of $\Delta_B P$ to be some pre-assigned universally applicable value $P_0 \neq 0$.

The exact character of the reference class of the local sets B is again inspired by comparability with completeness, We elect

[25] that the reference class of local recoil sets is, for each maximal integral curve Ω of the vector field X associated with the momentum P , the set of all intervals

of Ω of fixed¹⁸ length $d(\Omega)$.

The following precise formulation of classical global measurability can now be given.

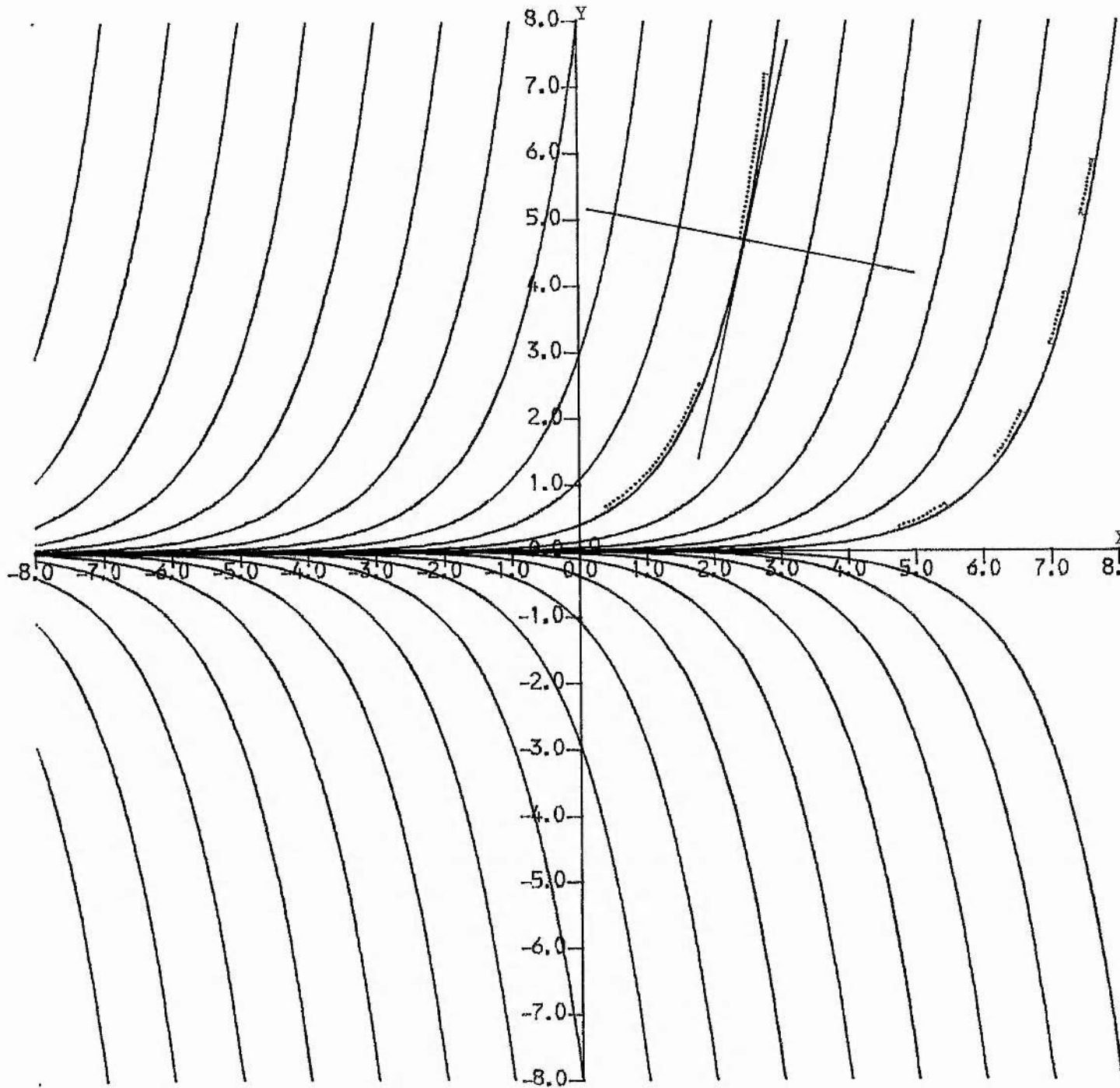
[26] A momentum P is classically globally measurable if and only if, for all maximal integral curves Ω of the associated vector field X , it is possible to elect a finite upper bound Δ_0 to the set of characteristic uncertainties $\Delta_B P$, standardized as in [24], and generated by the reference class [25] of local recoil sets B .

This is as illustrated in figure 2 overleaf. It will be noted that this final statement of classical global measurability is removed by a considerable margin from its original intuitive motivation in the idea of standard measurement, the reasons for this abstraction being largely connected with the need to admit as globally measurable as many momenta "having critical points" as possible. We shall defer the discussion of the link between local measurement and classical global measurability until §7, when we shall have in our possession the parallel concept of quantum global measurability.

Let us, for the present therefore, confine our attention to momenta P without critical points on M , and derive in this case the connection between completeness and global measurability. To this end we find it convenient to group together several properties of a maximal but incomplete integral curve of an incomplete vector field into the following theorem, the notation and results of which will be central in the subsequent discussion.

¹⁸ Note especially that the length $d(\Omega)$ can vary between integral curves and in particular need not exceed on every curve any fixed non-zero value. This variability is necessary to admit as globally measurable a large class of momenta whose vector fields possess critical points, and whose maximal integral curves can be of arbitrarily short length.

Figure 2: To illustrate the local recoil sets B_α within the reference class defined on the integral curves of a vector field.



The underlying graph is a family of maximal integral curves of the vector field $X = x\left(\frac{\partial}{\partial x}\right) + y\left(\frac{\partial}{\partial y}\right)$, which has a set of critical points $x=0$ which separates the flow into two distinct regions $x \geq 0$. We show along typical flow-lines of the vector field a representative group of local recoil sets B_α together with the local Cartesian coordinate directions (y^1, y^2) .

Theorem 10: On the properties of an incomplete maximal integral curve on a geodetically complete manifold.

Let (M, G, ρ) be a geodetically complete Riemannian manifold of metric tensor G and corresponding density ρ , and let the incomplete momentum P generate a C^∞ vector field on M , X , without critical points.

Let $s(\Omega, x, y)$, $x, y \in M$, denote the signed¹⁹ metrical distance along an arc Ω connecting x and y , and let $d(x, y)$, $x, y \in M$, denote the "true" distance between x and y , the unique distance along a minimal geodesic connecting them.

Let $x_0 \in M$ be a point on an incomplete maximal integral curve $\Omega(x_0)$, and define the covers, $\{\Omega^+(x_n), \Omega^-(x_n)\}$ of $\Omega(x_0)$ by

$$\Omega^+(x_n) = \{x \in M | x = \Phi_t(x_0), \tau^+ > t \geq t_n, \text{ where } t_n: x_n = \Phi_{t_n}(x_0)\}, \quad (57)$$

$$\Omega^-(x_n) = \{x \in M | x = \Phi_t(x_0), \tau^- < t \leq t_n, \text{ where } t_n: x_n = \Phi_{t_n}(x_0)\}, \quad (58)$$

where $\Phi_t: M \rightarrow M$ is the flow associated with the vector field X so defined that $\Phi_0(x_0) = x_0$, and where $(\tau^-, \tau^+) \neq \mathbb{R}$ is the range of the t -parameter on $\Omega(x_0)$.

Let $A \subset M$ denote a local set within M , and define the t -range of P through $x \in A$ by

$$R(x, A, P) = |\{t \in \mathbb{R} | \Phi_t(x) \in A\}|, \quad (59)$$

so that the t -range through $x \in A$ is simply the length $|b-a|$ of the interval (a, b) of t required to parameterize the segment of the integral curve $\Omega(x)$ contained within A .

Then we have the following properties.

¹⁹ If $\Omega = \Omega(x_0)$, then $s(\Omega, x, y) \geq 0$ if and only if $t(y) \geq t(x)$, where $x = \Phi_{t(x)}(x_0)$.

[27] $\Omega(x_0)$ neither is a closed curve nor has end points.

[28] The set $\Omega(x_0)$ is metrically infinite, and the sets $\Omega^+(x_0)$, $\Omega^-(x_0)$ semi-infinite, or symbolically

$$\forall \{t_n \geq 0\}_{n \in \mathbb{N}} \xrightarrow{\tau^+}, \{s(\Omega^+(x_0), x_0, \Phi_{t_n}(x_0))\} \rightarrow +\infty, \text{ and}$$

$$\forall \{t_n \leq 0\}_{n \in \mathbb{N}} \xrightarrow{\tau^-}, \{s(\Omega^-(x_0), x_0, \Phi_{t_n}(x_0))\} \rightarrow -\infty.$$

[29] If the sequence $\{x_n | n \in \Omega^+(x_0)\}_{n \in \mathbb{N}}$ is such that $\{s(\Omega^+(x_0), x_0, x_n)\} \rightarrow \infty$ and the associated sequence of t -values $\{t_n | x_n \in \Phi_{t_n}(x_0)\}_{n \in \mathbb{N}}$ is such that $\{t_n\} \rightarrow \tau^+ < \infty$, then the sequence of t -ranges $\{R(x_n, \Omega^+(x_n), P)\}_{n \in \mathbb{N}}$ tends to zero.

Proof: see appendix 7.

Consider now the reference class of local recoil sets $\{B_n | n \in \mathbb{N}\}$ defined as follows. Let $\Omega(x_0)$ be the incomplete maximal integral curve through $x_0 \in M$ of the incomplete vector field X associated with a momentum P without critical points. Select the subset, either $\Omega^+(x_0)$ or $\Omega^-(x_0)$, $\Omega^+(x_0)$ say²⁰, which has a finite t -range, therefore $[0, \tau)$, $\tau \in \mathbb{R}$, and define a sequence of points $\{x_n | n \in \mathbb{N}\} \subset \Omega^+(x_0)$ by $s(\Omega^+(x_0), x_0, x_n) = nd_0$, $d_0 \neq 0$. This sequence is infinite, since by [28] $\Omega^+(x_0)$ is semi-infinite in extent, and is "equally spaced" along $\Omega^+(x_0)$ of separation $d_0 = s(\Omega^+(x_0), x_{n-1}, x_n)$. We may now define the local recoil set B_n "centred" on x_n , in accordance with the requirement,

$$B_n = \{x \in \Omega^+(x_0) | -d_0 \leq s(\Omega^+(x_0), x_n, x) \leq d_0\}. \quad (60)$$

²⁰ If the t -range of $\Omega^+(x_0)$ is finite, replace P by $-P$ and X by $-X$ in the following argument.

Clearly these sets constitute a sub-class of the reference class of local recoil sets of $\Omega(x_0)$ defined in [25]. The crucial observation is that the sequence of characteristic (standardized) uncertainties $\{\Delta_{B_n} P\}_{n \in \mathbb{N}}$ associated with this sequence is, as is demonstrated in appendix 8, unbounded, that is that

$$\{\Delta_{B_n} P\}_{n \in \mathbb{N}} \rightarrow \infty, \quad (61)$$

so that we may immediately deduce the following theorem.

Theorem 11: On completeness and classical global measurability.

A momentum P , generating a vector field X without critical points on the manifold M , is classically globally measurable only if it is complete.

Proof: from (61) in contrapositive form.

§6: The Quantum Measurement of Momenta.

We address in this section the problem of the global measurement of a quantum momentum $Q(P)$. There naturally arise at least two essentially distinct procedures whereby some concept of localization within a finite region and therefore of local measurement may be introduced: we may seek either to introduce the idea of a local observable defined on $L^2_\rho(M)$, or else to restrict in some way the class of wave-functions so that the concept of localization lies in them. We elect to discuss these two approaches in turn.

§6.1: On the existence of local momenta.

The simplest means of introducing a "local" quantum attribute of a system employs the concept of a "local" observable. Such an observable may be characterized by the following properties.

[30] It is, without a certain locality, identically zero, so that no apparatus external to that region is required to determine its value.

[31] It agrees within that certain region with a global observable from which it is derived.

Let $A \subset M$ be a proper subset of M , which may be visualized as a small region of space around a point of M upon which an apparatus of sensitive volume A is constructed, and let π be the projector onto A by $\pi\psi = \chi(A)\psi$; then define the operator $Q_A^O(P)$ by,

$$Q_A^O(P) = \pi Q(P) \pi, \quad (62)$$

in which $Q(P)$ is the, unique, quantum momentum generated by the complete momentum P . Clearly $Q_A^O(P)$ is symmetric, since π and $Q(P)$ are self-adjoint of dense common domain, and moreover it obeys desideratum [30] trivially. However property [31] gives rise to difficulties since, in general, $DQ(P) \not\subset DQ_A(P)$, where $Q_A(P)$ is any self-adjoint extension of $Q_A^O(P)$, and hence a state possessing the global property $Q(P)$ may have no local attribute $Q_A(P)$ at all! Nevertheless when $\psi \in DQ_A(P) \cap DQ(P)$, $Q(P) = Q_A(P)$, so that [31] is at least proximately satisfied. There is a further difficulty with (62) however; for $Q_A^O(P)$ is, in general, neither self-adjoint nor essentially self-adjoint, and is thus a most uncertain candidate for an observable. All these points may be illustrated by a familiar example.

$$Q(P) = -i\hbar \frac{d}{dx}, \quad DQ(P) = \{\psi \in \mathcal{L}^2(\mathcal{R}) \mid \psi \in C^1(\mathcal{R}), Q(P)\psi \in \mathcal{L}^2(\mathcal{R})\}, \quad A = \mathcal{R}^+,$$

$$Q_A^O(P) = \pi \cdot -i\hbar \frac{d}{dx} \pi, \quad DQ_A^O(P) = \{\psi \in \mathcal{L}^2(\mathcal{R}) \mid \pi\psi \in C^1(\mathcal{R}), \pi Q(P)\pi\psi \in \mathcal{L}^2(\mathcal{R})\}$$

An argument based on the standard analysis²¹ of $-i\hbar \frac{d}{dx}$ on \mathcal{R}^+ shows that $Q_A^O(P)$ is a maximal symmetric operator, but is neither self-adjoint nor essentially self-adjoint.

²¹ see Akhizer and Glasman⁽²⁵⁾ where this is discussed in detail.

Resuming our discussion we consider the source of the violation of the condition $DQ(P) \subseteq DQ_A(P)$. Clearly if $Q(P)\psi \in \mathcal{L}_\rho^2(M)$ then, if defined, $\pi Q(P)\pi\psi \in \mathcal{L}_\rho^2(M)$; hence the problem arises from the violation of the domain constraints,

$$\psi \in C^1(X, M), \pi\psi \in C^1(X, M), \quad (62)$$

where X is the vector field associated with the momentum P .

In general, $\psi \in C^1(X, M)$ does not imply $\pi\psi \in C^1(X, M)$, unless when ψ or $X\psi \rightarrow 0$ as $x \rightarrow \partial A$, the boundary of A . Now the condition $X\psi \rightarrow 0$ as $x \rightarrow \partial A$ can be satisfied without constraint of ψ only if $X \rightarrow 0$ as $x \rightarrow \partial A$, so that the X -flow "stagnates" as $x \rightarrow \partial A$, and thus A is invariant under the flow of X . This statement is equivalent to the completeness of the restriction $X|_A$ of X to A , so that we anticipate that only those sets A which are invariant under the flow of X will possess the desiderata [30] and [31] above. That this is indeed the case is contained in the following theorem.

Theorem 12: On the existence of local momenta.

Let X be a complete C^∞ vector field on M , generated by a momentum P , and let $Q(P)$ be the quantum observable associated with P ; then the operator $Q_A^O(P) = \pi Q(P)\pi$, formed from the projector π of M onto A , is essentially self-adjoint if and only if A is invariant under the flow of X . The unique self-adjoint extension of such a $Q_A^O(P)$, $Q_A(P)$, the local quantum momentum in A , can be given explicitly as,

$$Q_A(P) = [Q_A^O(P)]^\dagger, \quad (64)$$

where $Q_A(P)$ has differential expression

$$Q_A(P) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) \chi(A), \quad (65)$$

and domain of definition

$$DQ_A(P) = \{\psi \in \mathcal{L}^2_\rho(M) \mid Q_A(P)\psi \in \mathcal{L}^2_\rho(M)\} . \quad (66)$$

Proof: see appendix 9.

The principal difficulty lies in the restricted sense in which the $Q_A(P)$ of theorem 12 may be considered "local". It is, in general, not possible to define a $Q_A(P)$ on an arbitrarily pre-elected region A of M , so that an apparatus whose sensitive volume is A cannot be associated with a suitable local operator; equally a "local" observable of non-zero domain A cannot, in general, be measured by an apparatus since the extent of the region A may be metrically very large or even infinite. It follows, therefore, that an alternative method of describing the local behaviour of observables must be sought in the general case, but, before proceeding to do so, we establish explicitly the link between the well-formed "local" observables and the global observable from which they are derived.

Theorem 13: On the reconstruction of a global momentum.

Let $\{Q_{A_\alpha}(P)\}$ be a family of well-defined local observables generated from the global observable $Q(P)$ by $Q_{A_\alpha}(P) = [\pi_\alpha Q(P) \pi_\alpha]^\dagger$, such that $\{A_\alpha\}$ forms a partition of M ; then we have the identity,

$$Q(P) = \sum_\alpha Q_{A_\alpha}(P) . \quad (67)$$

Proof: see appendix 9.

§6.2: Uncertainty and measurability.

Having ascertained that local momentum observables cannot, with any degree of generality, be defined in accordance with the desiderata [30] and [31] above, without restriction of the class of wave functions upon which local measurements may be performed, we consider in this

section some consequences of an attempt to admit local measurement by such a restriction. The elected set of admissible wave functions must both be sufficiently narrow as to admit of localizability and yet sufficiently broad to allow the accurate measurement of momentum. But it is at the heart of quantum mechanics that these two concepts, knowledge of position and knowledge of momentum, are, in a sense, mutually exclusive, as is embodied in the Principle of Uncertainty. It is clear, therefore, that this fundamental uncertainty will be central to the discussion of quantum measurability. It is this relationship which will lead us again to the concept of completeness as a necessary condition for global measurability.

We first address the problem of defining the form of the Uncertainty Principle appropriate to a metrically finite, non-zero, region A of M , within which we seek to determine the momentum P . We shall assume that

[32] there exists a local chart $\{x^i | i \in [1, n]\}$ covering A on which P has the canonical coordinatization p_1 ;

then, since the pair (x^1, p_1) is canonically conjugate, it is clear that the desired Uncertainty Principle will be constructed upon the quantum analogues, $Q(x^1)$, $Q(p_1)$. However neither $Q(x^1)$ nor $Q(p_1)$ can be simply defined as a self-adjoint operator over M , so that their definitions, conditions for existence, and meaning need be separately discussed.

The chart $\{x^i | i \in [1, n]\}$ is, in general²², non-global, so that x^1 is not well defined outwith a subregion of M . However we may define a global observable in accordance with the desideratum [30] of §6.1 by the expression,

²² Where $\{x^i | i \in [1, n]\}$ is global, we may also define $\tilde{Q}(x^1) = x^1$, $D\tilde{Q}(x^1) = \{\psi \in \mathcal{L}^2_\rho(M) | \tilde{Q}(x^1)\psi \in \mathcal{L}^2_\rho(M)\}$. It is clear that $Q(x^1)$ as defined in (68), (69), is the local observable generated by the global operator $\tilde{Q}(x^1)$ within the region A .

$$Q(x^1) = x^1 \chi(A) , \quad (68)$$

(which is to be interpreted as a function on $\mathcal{L}_\rho^2(M)$ whose expression within A coincides with the coordinate function $x^1(x)$, and outwith A , $\chi(A)$ being the characteristic function of A , is zero identically), and by the domain of definition,

$$DQ(x^1) = \{\psi \in \mathcal{L}_\rho^2(M) \mid Q(x^1)\psi \in \mathcal{L}_\rho^2(M)\} . \quad (69)$$

$Q(x^1)$, being self-adjoint, global, and reducing to x^1 on A , is clearly the natural quantum analogue of x^1 .

If x^1 is not global, then p_1 is not defined everywhere on M ; however, since p_1 is the local representation of the global momentum P , the natural quantum analogue $Q(p_1)$ of p_1 is formed by $Q(P)^{23}$ whenever this latter exists. As was discussed in §3, the operator $Q(P)$ is a self-adjoint extension of a uniquely determined operator $Q_0(P)$. Three possible situations may arise;

[33] $Q_0(P)$ may have no self-adjoint extensions, when $Q(P)$ clearly does not exist. However we may nevertheless define an Uncertainty Principle by restricting the class of admissible wave-functions to a suitable subset of $C_0^\infty(M)$, when we may interpret $Q(P)$ as being simply the symmetric operator $Q_0(P)$.

[34] $Q_0(P)$ may have many self-adjoint extensions of which at most one may be $Q(P)$; (we assume that such a unique $Q(P)$ does indeed correspond to the quantum momentum, although its exact domain of definition is unknown.)

[35] $Q_0(P)$ has a unique self-adjoint extension equal to $Q(P)$ and defined by (5) and (6).

²³ for in general no local observable $Q_A(P)$ will exist defined on A .

In every case, we construct the commutator of $Q(x^1)$ and $Q(P)$ to deduce,

$$[Q(x^1), Q(P)] = -i\hbar \chi(A) . \quad (70)$$

Hence we deduce, following the standard manipulation²⁴, the derived form of the Uncertainty Principle,

$$\Delta Q(x^1) \Delta Q(P) \geq \frac{\hbar}{2} p(A) , \quad (71)$$

in which $p(A) = \langle \psi | \chi(A) | \psi \rangle$ is the probability that a particle endowed with the momentum $Q(P)$ will be found in A . The domain of functions ψ to which (71) applies is as yet unknown, since the domain of $Q(P)$ is, in general, unknown; however whatever the exact form of $DQ(P)$, we may define an explicitly known subset of the commutator domain by,

$$\mu_o(A, P) = \{ \psi \in C_o^\infty(M) | \chi(A)\psi \in C_o^\infty(A) \} . \quad (72)$$

The set $\mu_o(A, P)$ consists of, in a sense, "ideal" wave functions; for not only do they obey the Uncertainty Principle above, but also an apparatus may be constructed where sensitive volume A encloses a maximally connected subregion of their support, and may certainly, therefore, be used to measure the local momentum values within A .

Consider now the progress of a momentum measurement conducted wholly within the set A . Two aspects of the local measurement may be noted;

[36] no account is taken of position or momentum values
outwith A , and

[37] the measuring device of sensitive volume A will
record the momenta only of these particles perceived
immediately before the measurement as lying within A .

²⁴ see, say, Roman⁽²⁶⁾, and note that all that is required is that $Q(P)$ be symmetric.

These features imply that the local apparatus records a spectrum of values from the state

$$\psi(A) = p^{-\frac{1}{2}}(A) \chi(A) \psi, \quad p(A) \neq 0, \quad (73)$$

which results from the projection²⁵ into the set A of the original wave function $\psi \in \mu_0(A, P)$ describing an ensemble of particles in M.

It is clear, therefore, that, whatever the means of the actual momentum determination, the standard deviations of the local position and momentum measurements within A are subject to the fundamental inequality, obtained from (71) and (73),

$$\Delta_A Q(P) \Delta_A Q(x^1) \geq \frac{\hbar}{2}, \quad p(A) \neq 0, \quad (74)$$

the condition $p(A) \neq 0$ requiring simply that particles bearing the momentum P do in fact manifest themselves within A.

Observe that this last equation, which is the kernel of our analysis of local quantum measurement, does not depend for its validity upon the considerations of [36] and [37], and in particular upon the projection postulate embodied in (73); but may be alternatively derived by means of an a priori restriction of the class of admissible state functions to the set $C_0^\infty(A)$. The above analysis is, therefore, to be regarded as an attempt to avoid so drastic a restriction of the class of admissible states, so as to admit the measurement by a local apparatus of as large a class of states as is possible.

It is possible, moreover, to determine an upper bound to the standard deviation $\Delta_A Q(P)$ associated with a state ψ of the system, and hence a lower bound to the greatest available locally repeatable accuracy $\Delta_A Q(P)$ of a momentum measurement. For, through every $x \in A$ there is a uniquely defined t-range of P given as in (59) by $R(x, A, P)$,

²⁵ We assume here for definiteness that Ludder's⁽²⁷⁾ projection postulate is valid.

which, since the flow-parameter t along every integral curve of P within A is, to within an additive constant, simply²⁶ the coordinate variable x^1 of the local canonical chart, can be identified with the maximum range $R(A, P)$ of the coordinate x^1 within A , so that we have

$$R(A, P) = \sup_{x \in A} R(x, A, P) . \quad (75)$$

Further, since for any state $\psi \in \mu_0(A, P)$ the standard deviation $\Delta_A Q(q^1)$ is bounded above by $R(A, P)$, we have in complete generality,

$$\Delta_A Q(P) \geq \frac{\hbar}{2} 1/\Delta_A Q(q^1) \geq \frac{\hbar}{2} R^{-1}(A, P) . \quad (76)$$

Having completed our discussion of local observation, we now consider the problem of the global measurement of a momentum P . We shall, in the foregoing, assume that the Riemannian manifold (M, G) over which the momentum is defined is geodetically complete. This choice, parallel to the corresponding classical analysis, assures by virtue of the following theorem, the well-definedness of the free quantum Hamiltonian $Q(H)$.

Theorem 14: On the existence of the quantum free Hamiltonian.

The symmetric operator $Q_0(H)$ defined by

$$Q_0(H) = - \frac{\hbar^2}{2m} \nabla^2 , \quad (77)$$

on the domain

$$DQ_0(H) = \{ \psi \in \mathcal{L}_p^2(M) \mid \psi \in C_0^\infty(M), Q_0(H)\psi \in \mathcal{L}_p^2(M) \} , \quad (78)$$

²⁶ In terms of the canonical chart $\{x^i \mid i \in [1, n]\}$, $\Phi_t(x^1, x^2, \dots, x^n) = (x^1 + t, x^2, \dots, x^n)$.

is essentially self-adjoint if the manifold (M,G) is geodetically complete.

Proof: see Abraham and Marsden⁽²⁸⁾, Chernoff⁽²⁹⁾.

We next introduce the concept of quantum global measurability, the intuitive motivation of which is analogous to that of classical global measurability, the concept being based upon a comparison within a given reference class of appropriately standardized characteristic uncertainties $\Delta_A Q(P)$.

Firstly we eliminate from the $\Delta_A Q(P)$ any state-dependence by so standardizing that

[38] we compare only the least standard deviations,

$$\inf_{\psi \in \mu_O(A,P)} \Delta_A Q(P).$$

It is readily seen that the corresponding maximal uncertainty in the values of x^i is given by

$$\sup_{\psi \in \mu_O(A,P)} \Delta_A Q(q^i) = R(A,P), \quad (79)$$

which result clearly reflects the importance of equation (76).

Secondly we elect for each maximal integral curve Ω of the vector field X associated with P the set of all local sets A in accord with the following requirements as the reference class of local sets constructed over Ω .

[39] The set A needs to contain a point $x \in \Omega$ such that

$$A \cap \Omega = \{y \in \Omega \mid -d(\Omega) \leq s(\Omega, x, y) \leq d(\Omega)\}, \quad (80)$$

where $d(\Omega)$ may vary between different integral curves, and

[40] The maximum t -range within A must equal the t -range within $\Omega \cap A$, or symbolically

$$R(A, P) = R(x, A, P) = R(A \cap \Omega, P) . \quad (81)$$

A precise formulation of the concept of quantum global measurability can now be given.

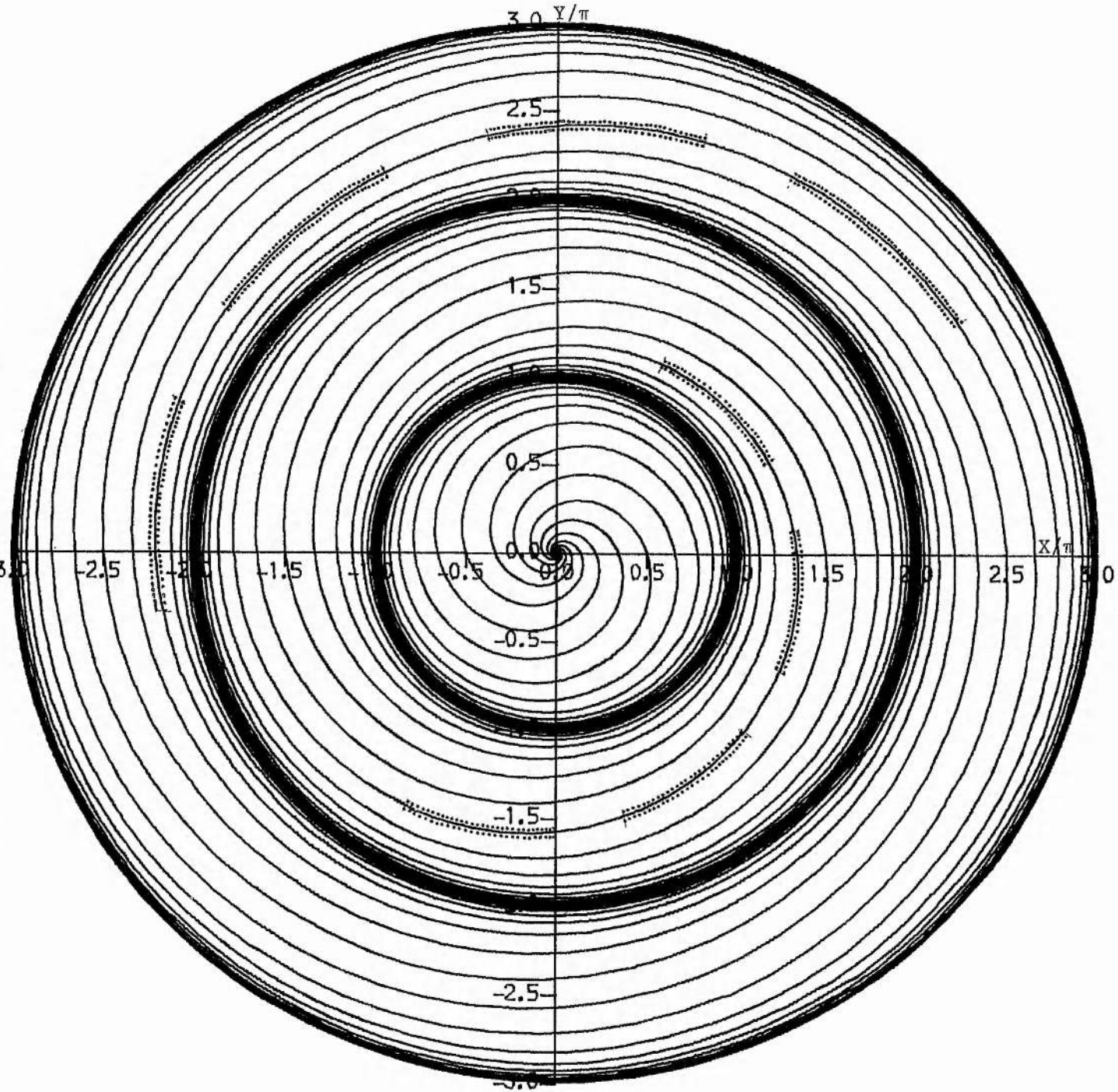
[41] A momentum P is quantum globally measurable if and only if, for all maximal integral curves Ω of the associated vector field X , it is possible to elect a finite upper bound Δ_0 to the set of least characteristic uncertainties $\Delta_A Q(P)$, generated from the reference class of local sets A constructed over Ω in accord with [39] and [40].

The construct described above is illustrated in figure 3 overleaf.

We now proceed to discuss in the case of a momentum P without critical points the link between quantum global measurability and completeness. We elect, parallel to the corresponding discussion of classical global measurability, a sequence of sets $\{A_n | n \in N\}$ as follows. Let $\Omega(x_0)$ be the incomplete maximal integral curve of X associated with P through some suitably chosen $x_0 \in M$, of which we select the subset, $\Omega^+(x_0)$ say, which has a finite t -range $[0, \tau^+)$, $\tau^+ \in \mathcal{R}$. Define the (infinite) sequence of points $\{x_n | n \in N\} \subset \Omega^+(x_0)$ by $s(\Omega^+(x_0), x_0, x_n) = nd_0$, $d_0 \neq 0$. By identifying each x_n with the particular $x \in A_n$ of condition [39], and by imposing upon each set A_n the demand [40], we ensure that the class of sets $\{A_n | n \in N\}$ is contained in the reference class of local sets over $\Omega(x_0)$. The crucial observation is that, as is immediate from the result [29] of theorem 10,

$$\{R(A_n, P)\}_{n \in N} \rightarrow 0 \text{ as } n \rightarrow \infty , \quad (82)$$

Figure 3: To illustrate the choice of the local sets A_α within the reference classes defined in the concept of quantum global measurability.



The underlying graph is the family of maximal integral curves of the vector field given in polar coordinates by $X = \sin r \frac{\partial}{\partial r} + 2 \frac{\partial}{\partial \theta}$, which has a critical point at $(0,0)$. The flow is confined to annular regions by the circular integral curves $r = n\pi$, $n \in \mathbb{N}$. Some representative local sets A_α have been drawn on two typical integral curves.

so that the sequence of least characteristic uncertainties generated by the sets A_n is unbounded. That is, since (76) yields the equality

$$\inf_{\psi \in \mu_0(A,P)} \Delta_{A_n} Q(P) = \frac{\hbar}{2} R^{-1}(A_n, P), \quad (83)$$

we have

$$\left\{ \inf_{\psi \in \mu_0(A_n, P)} \Delta_{A_n} Q(P) \right\} \rightarrow \infty \text{ as } n \rightarrow \infty. \quad (84)$$

The above analysis embodies the proof of the final theorem of this section.

Theorem 15: On completeness and quantum global measurability.

A momentum P , generating a vector field X without critical points on M , is quantum globally measurable only if it is complete.

Proof: this follows from (84) in contrapositive form.

§7: On Classical and Quantum Global Measurability.

Our aim in this section will be to outline some of the characteristics of quantum and classical global measurability. We first illustrate by explicit calculation upon two representative momenta the procedure involved in the determination of whether a given momentum is classically or quantum globally measurable, then discuss briefly some features of the definition of global measurability, and finally obtain some general results which will illuminate the character of globally measurable momenta.

§7.1: Two illustrative examples on the global measurability of momenta.

[42] The angular momentum observable L_z on the Euclidean plane.

In terms of global Cartesian coordinates (x, y) defined on the Euclidean plane \mathbb{R}^2 with the usual metric, and the corresponding chart (x, y, p_x, p_y) of $T^*\mathbb{R}^2$, L_z assumes the familiar form

$$L_z = xp_y - yp_x, \quad (85)$$

and is associated with the C^∞ complete vector field

$$X = x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}, \quad (86)$$

whose maximal integral curves are given parametrically in terms of the flow-maps $\Phi_t: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ by

$$\Phi_t(x, y) = (x \cos t - y \sin t, x \sin t + y \cos t), \quad (87)$$

the integral curves of X forming a concentric family of circles of centre $(0, 0)$. The canonical coordinates associated with L_z , in terms of which X assumes the canonical form $\frac{\partial}{\partial \theta}$ and the metrical line element $ds^2 = dx^2 + dy^2$ the form $dr^2 + r^2 d\theta^2$, are simply the (almost global) plane polar coordinates (r, θ) defined on the cut-plane in the usual manner.

The maximal integral curves of X , and a representative grid of the polar coordinate system are displayed in figure 4.

We now determine whether or not L_z is classically globally measurable. Let us first introduce, for a representative integral curve Ω defined by

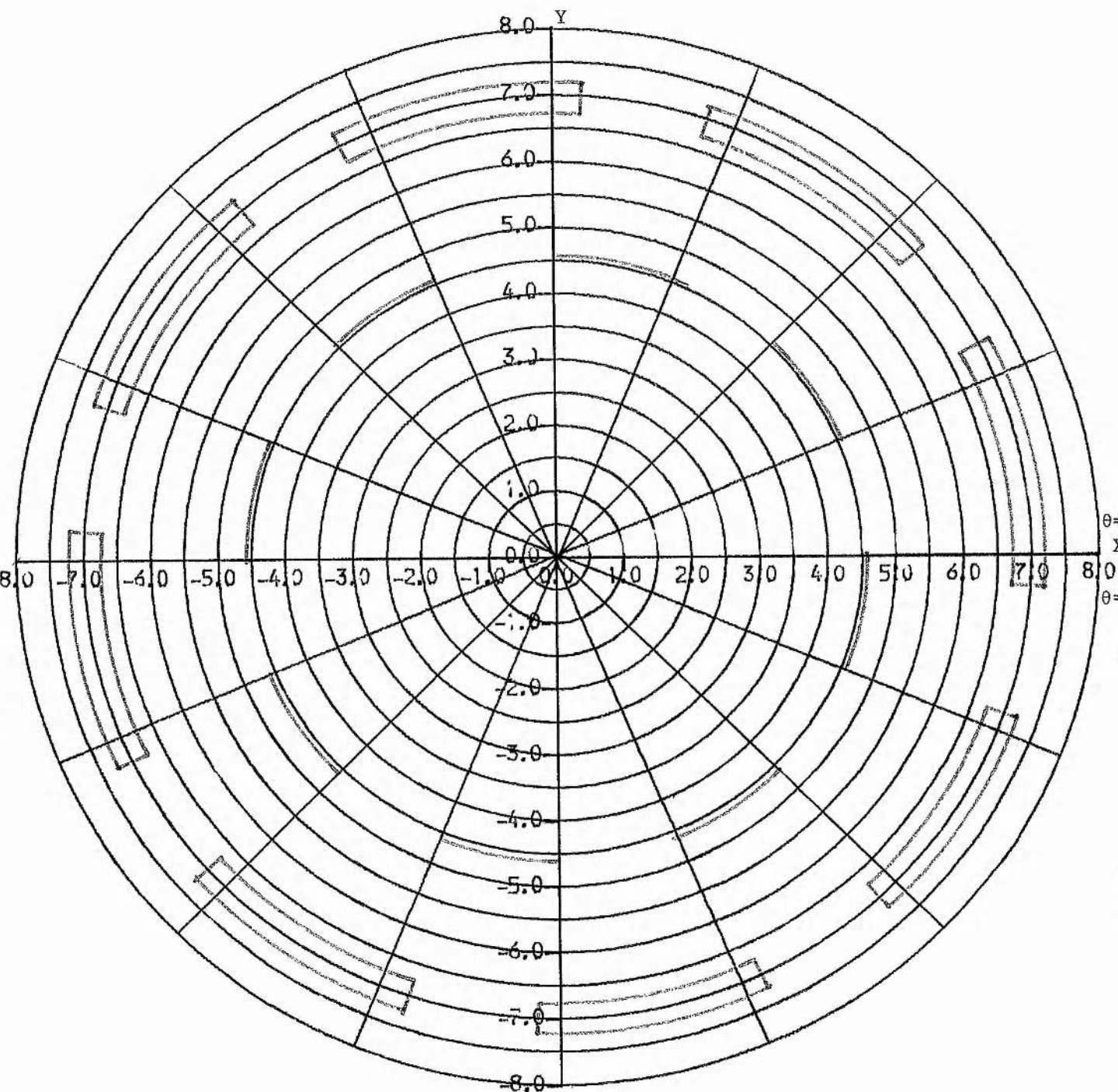
$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid r = a > 0\}, \quad (88)$$

an associated reference class $\{\beta_\alpha \mid \alpha \in [0, 2\pi)\}$ of local recoil sets B_α defined in accordance with the requirement [25] by

$$B_\alpha = \{(x, y) \in \Omega \mid -d_0/2 \leq s(\Omega, (a \cos \alpha, a \sin \alpha), (x, y)) \leq d_0/2\}, \quad (89)$$

in which $0 < d_0 \leq 2\pi a$ is the (metrical) length of a typical local recoil set B_α .

Figure 4: To illustrate the maximal integral curves of L_z , and a representative grid of the polar coordinate system (r, θ) .



We also illustrate on the figure some typical local recoil sets B_α as defined in equation (89), and some local sets A_α of equation (93).

The branch cut in the coordinate system is the radius $\{(x, y) | y = 0, x \geq 0\}$.

Next we observe that we may introduce along each arc Ω an alligned Cartesian coordinate $s(\theta)$ defined by $s = a\theta$, in terms of which the vector field X assumes the form $X = a\partial/\partial s$. It is now immediate that the function $b_1^1(x)$ on Ω is simply

$$b_1^1(x, y) = a, \quad (90)$$

and that, in accordance with the definitions of formulae (53) and (54), the measured value of L_z within the recoil set B_α is

$$P = aP_0, \quad (91)$$

with an associated characteristic error

$$\Delta_{B_\alpha} P = 0. \quad (92)$$

It will now be apparent that L_z is indeed classically globally measurable. It is remarkable, moreover, that it is possible to measure L_z without error $\Delta_{B_\alpha} P$ within every recoil set B_α , a result which clearly reflects the rather special character of the angular momentum observable.

Let us finally consider the question of whether L_z is quantum globally measurable. To answer this question let us introduce, for a typical integral curve Ω as above, the corresponding reference class $\{A_\alpha | \alpha \in [0, 2\pi)\}$ of local sets A_α defined in accordance with the requirements [39] and [40] by the prescription,

$$A_\alpha = \{(x, y) \in \mathbb{R}^2 | (x, y) = \Phi_\alpha(x_0, y_0), (x_0, y_0) \in A_0\}, \quad (93)$$

$$A_0 = \{(x, y) \in \mathbb{R}^2 | 0 < a - d_1/2 \leq r \leq a + d_1/2, \theta \in (0, d_0/a \leq 2\pi)\}.$$

Each set A_α , obtained by a rotation of the set A_0 through an angle α about the origin of coordinates is "cuniform" of θ -span d_0/a and r -span d_1 as illustrated. It is now immediate that $R(A_\alpha, P) = d_0/a$, and therefore that the least uncertainty $\Delta_{A_\alpha} Q(P)$ in the A_α -local momentum

measurement is simply

$$\Delta_{A_\alpha} Q(P) = \frac{\hbar a}{2d_0}, \quad (94)$$

so that L_z is also quantum globally measurable.

Note that, while the characteristic least uncertainty $\hbar a/2d_0$ in an A_α -local measurement of $Q(L_z)$ is independent of the exact location of A_α on Ω , it is nevertheless, in contradistinction to the classical error $\Delta_{B_\alpha} P$, never zero, and indeed increases without limit as d_0 is reduced to zero. This is as would be anticipated from a naïve application of the uncertainty principle.

[43] The observable $P_1 = (x+y)p_x - (x-y)p_y$ on the Euclidean plane.

Consider the momentum P_1 defined in terms of global Cartesian coordinates of \mathbb{R}^2 , and the corresponding chart of $T^*\mathbb{R}^2$ by the prescription

$$P_1 = (x-y)p_x + (x+y)p_y. \quad (95)$$

This momentum is associated with a C^∞ complete vector field

$$X = (x-y) \frac{\partial}{\partial x} + (x+y) \frac{\partial}{\partial y}, \quad (96)$$

whose maximal integral curves are given parametrically in terms of the maps $\Phi_t: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ by

$$\Phi_t(x,y) = e^t(x \cos t - y \sin t, x \sin t + y \cos t), \quad (97)$$

and are represented geometrically as spirals radiating from the critical point of X at the origin of coordinates. A set of canonical coordinates associated with P_1 , in terms of which X assumes the form $\partial/\partial\phi$ and the metrical line-element ds^2 the form $\exp(\phi+\psi)(d\phi^2+d\psi^2)$, may be defined in terms of the almost global plane polar coordinate (r,θ) by the equations,

$$\phi = \frac{1}{2}(\ln r + \theta), \quad \psi = \frac{1}{2}(\ln r - \theta), \quad (98)$$

in which we take for definiteness $\theta \in [0, 2\pi)$.

Some maximal integral curves of X , and a representative grid of the coordinates (ϕ, ψ) are displayed in figure 5.

Introduce on each maximal integral curve

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid \psi = \psi_0\}, \quad (99)$$

a coordinate $s(\phi)$ defined by

$$s(\phi) = \int_{-\infty}^{\phi} \exp \frac{1}{2}(\phi + \psi_0) d\phi = 2 \exp(\frac{1}{2}(\phi + \psi_0)), \quad (100)$$

which measures the (metrical) distance from the critical point of X to the point (ϕ, ψ_0) of Ω , and in terms of which the function $b_1^1(x)$ on Ω assumes the form

$$b_1^1(s) = \frac{ds}{d\phi} = \frac{1}{2}s. \quad (101)$$

This completes the discussion of technical preliminaries.

Turning now to the question of the classical global measurability of P_1 , we introduce, for a representative integral curve Ω , an associated reference class $\{B_\alpha \mid \alpha \geq d_0/2\}$ of local recoil sets B_α defined in accordance with [25] by

$$B_\alpha = \{(x, y) \in \Omega \mid 0 \leq -d_0/2 + \alpha \leq s(\phi) \leq \alpha + d_0/2\}, \quad (102)$$

where the auxiliary condition $\alpha \geq d_0/2$ simply ensures that a set of length d_0 can be centred on $(s, \psi) = (\alpha, \psi_0)$.

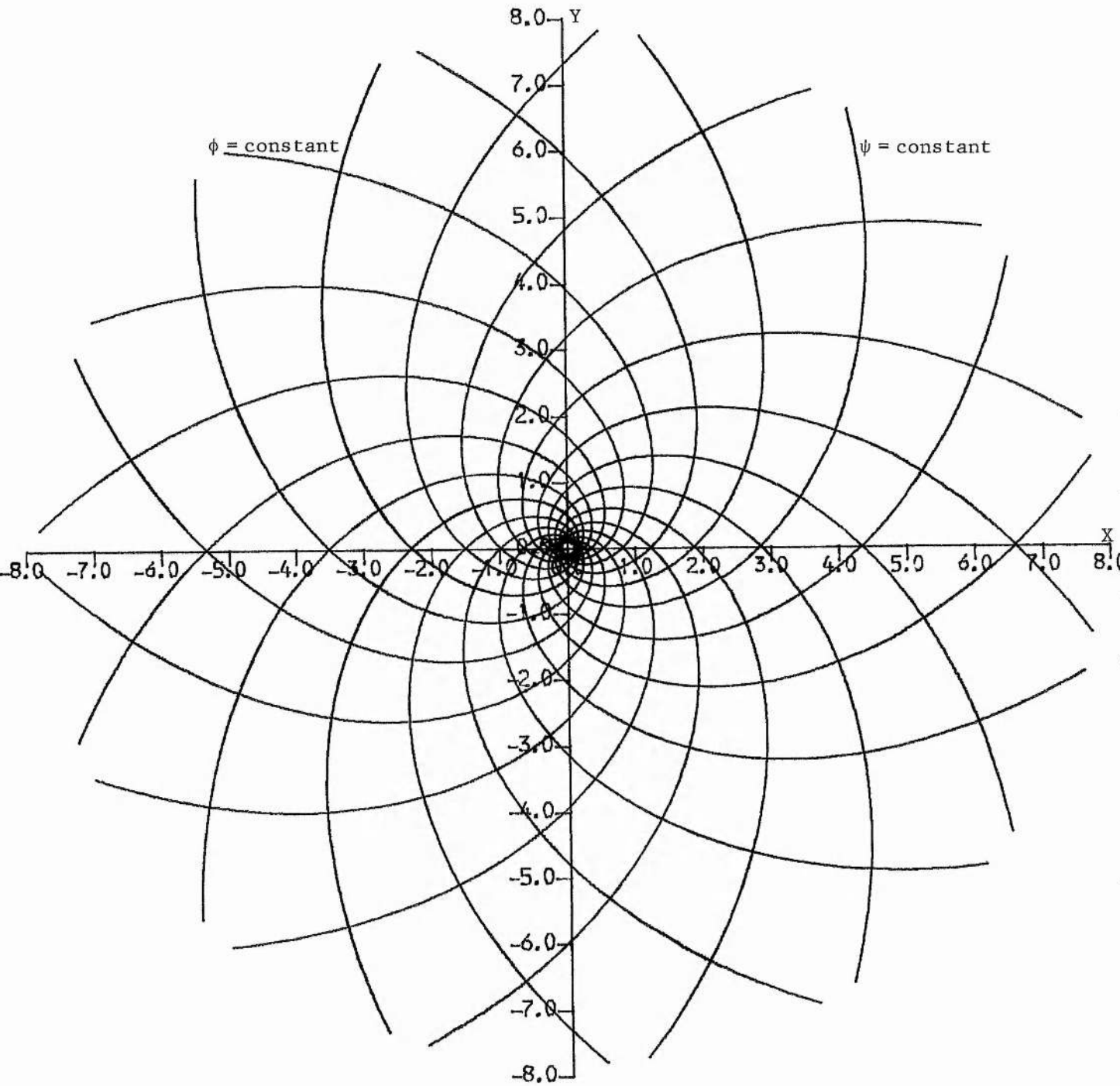
It is now elementary to confirm that the local value of P_1 in B_α is simply

$$P = b_1^1(B_\alpha)P_0 = \frac{1}{2}\alpha P_0, \quad (103)$$

and that the associated characteristic error is

$$\Delta_{B_\alpha} P = \frac{1}{4\sqrt{3}} d_0, \quad (104)$$

Figure 5: To illustrate the maximal integral curves of the momentum P_1 , of corresponding vector field $X = (x-y) \frac{\partial}{\partial x} + (x+y) \frac{\partial}{\partial y}$.



The maximal integral curves of X are the marked counterclockwise spirals emanating from the origin of coordinates, the second family being a representative set of coordinate surfaces perpendicular to the integral curves of X . The equations of the arcs are

$$\phi = \frac{1}{2}(\ln r + \theta), \quad \psi = \frac{1}{2}(\ln r - \theta), \quad \theta \in [0, 2\pi).$$

so that P_1 is indeed classically measurable.

We may note that the characteristic errors in this case, while non-zero, are nevertheless independent of the sets B_α , and even of the integral curves Ω , so that, if d_0 is given, $1/48 d_0^2$ marks a universally applicable characteristic error in the local measurement of P_1 .

Finally, addressing the problem of the quantum global measurability of P_1 , we introduce, for a typical Ω as above, a corresponding (exhaustive) reference class $\{A_\alpha | \alpha \geq d_0/2\}$ of local sets A_α defined in accordance with the requirement [40] and the prescription

$$A_\alpha \cap \Omega = B_\alpha. \quad (105)$$

It follows from (100) that the range of ϕ within A_α is given by

$$R(A_\alpha, P) = 2 \ln \left[\frac{2\alpha + d_0}{2\alpha - d_0} \right], \quad (106)$$

and hence that the least characteristic uncertainty $\Delta_{A_\alpha} Q(P)$ is given by

$$\Delta_{A_\alpha} Q(P) = \frac{\hbar}{4} \ln^{-1} \left[\frac{2\alpha + d_0}{2\alpha - d_0} \right] \rightarrow \infty \quad \text{as} \quad \alpha \rightarrow \infty. \quad (107)$$

It is now clear that P_1 is not quantum globally measurable, and that the converse of theorem 15 is, in general, false.

We close this section by considering briefly the definitions of classical and quantum global measurability in the light of the example [42] developed above, and isolate for justification the following two features of the definitions;

[44] the demand, embodied in [26] and [41] above, that

upper bounds $\Delta_0(\Omega)$ should exist only for each integral curve Ω of the vector field X associated with momentum P , rather than the demand that a global upper bound Δ_0 should exist for all integral curves of the vector field, $\Delta_0 = \sup_{\forall \Omega} \Delta_0(\Omega)$, and

[45] the admitted variability of the characteristic length $d(\Omega)$ of [25] and [39] between different integral curves of the vector field X associated with P .

Consider firstly the demand [44]. For a quantum measurement of L_z within a local set A_α over the integral curve $\Omega = \{(x, y) | x^2 + y^2 = a^2 \neq 0\}$, the characteristic uncertainty in the momentum value is simply $\Delta_{A_\alpha} Q(P) = \hbar a / 2d_0$, so that, to obtain a global upper bound $\Delta_0 = \sup\{\forall \alpha, \hbar a / 2d_0\}$, it would be necessary to specify the relationship to be assumed between d_0 and a , clearly a task which admits, for a general momentum, of no obvious solution. This difficulty is most readily solved simply by restricting our attention to each integral curve Ω of X , when no conditions need be imposed on $d(\Omega)$, else these analogous to the constraint $d_0 \leq 2\pi a$ of L_z .

Similarly the justification of [45] is also inherent in the above analysis; for we must have $d_0 \leq 2\pi a$ so that if a global characteristic length $d_0 = \inf d(\Omega)$ is to be chosen, we must have $d_0 \leq \inf\{\forall a, 2\pi a\} = 0$, which contradicts the requirement that $d_0 \neq 0$.

§7.2: On exact classical global measurability.

Having observed that neither all complete, nor all classically globally measurable, momenta are quantum globally measurable, we now enquire: Is it possible to identify a physically important subclass of the complete momenta which are both classically and quantum mechanically globally measurable?

To this end we introduce a refinement of the idea of classical global measurability as follows.

[46] A momentum P is exactly classically globally measurable if and only if, for every local recoil set B_α which is a subinterval of a maximal integral curve Ω of the vector field associated with P , the characteristic local error

$\Delta_{B_\alpha} P$ satisfies

$$\Delta_{B_\alpha} P = 0. \quad (108)$$

This concept is motivated partly by the observation that L_z satisfies (108), but principally by the recognition of the uniquely privileged character of these momenta in being globally measurable "without error". The link with quantum global measurability is now immediate.

Theorem 16: On exact classical and quantum global measurability.

If a momentum P is exactly classically globally measurable then it is quantum globally measurable²⁷.

Proof: see appendix 10.

Thus we see that the exactly classically globally measurable momenta do indeed define a subclass of the complete momenta furnishing an answer to the above posed question provided only that we can show that some physically important momenta are, as a class, exactly classically globally measurable, a result comprising the following theorem.

Theorem 17: On Killing momenta and exact classical global measurability.

Every complete Killing momentum P , defined by the requirement that its associated vector field X is Killing⁽³⁰⁾, is exactly classically globally measurable, and is moreover quantum globally measurable.

Proof: see appendix 10.

²⁷ In fact every exactly classically globally measurable momentum P is "optimally" quantum globally measurable; that is that the characteristic least error $\Delta_{A_\alpha} Q(P)$ associated with a quantum measurement of P in A_α , depends only upon the length $d(\Omega)$ of A_α and upon the particular integral curve Ω over which A_α is defined, but does not depend upon the exact location on Ω of A_α . (cf (94) above.)

This result is surely a most powerful affirmation of the importance of the concepts of classical and quantum global measurability. Before proceeding to the conclusion of this chapter, we introduce in the form of a theorem, a postscript upon exact classical global measurability.

Theorem 18: Alternative formulations of exact classical global measurability. L.

Let P be a complete momentum over the Riemannian manifold (M, G) , and let $\{x^i | i \in [1, n]\}$ be a local canonical coordinate system in terms of which the vector field X associated with P becomes $\partial/\partial x^1$.

Then P is exactly classically globally measurable if and only if either

[47] for every maximal integral curve $\Omega(s)$ of X , parameterised by an arc-length parameter s , $b_1^1(s)$ is constant along $\Omega(s)$,

or

[48] for every local canonical chart $\{x^i | i \in [1, n]\}$, the metric tensor $g_{ij}(x^k)$ satisfies

$$\frac{\partial g_{11}}{\partial x^1} = 0 . \quad (109)$$

Proof: see appendix 10.

§8: Conclusion and Prospect.

The analysis of the foregoing sections have identified two severe difficulties associated with the retention of the incomplete momenta as quantizable objects,

[49] the absence of any uniquely and explicitly known procedure for their quantization, and

[50] their global immeasurability, either classically or quantum mechanically,

these two features being associated with complementary aspects of the process of subjecting the theory to experimental test. Neither of these problems is encountered in the case of complete, classically, and quantum globally measurable momenta.

We wish to stress that the objections we have raised against the incomplete momenta are based upon their global properties: in particular we do not claim, contrary to established practice, that the incomplete momenta have no local meaning, and indeed it may be that they are very useful in discussing local physical effects²⁸.

However, notwithstanding these remarks concerning the local significance of an incomplete momentum, it remains true that any fully acceptable observable must be globally well defined.

We, therefore, tentatively propose the following axiom of quantizability:

²⁸ This observation affords an area of possible extension of the work of this chapter, based upon the following consideration. Let $A \subset M$, a metrically finite subset of M of compact closure \bar{A} , denote a local set within the manifold M , and let $\psi \in \{\psi \in \mathcal{L}^2_p(M) \mid \psi \in C^\infty_0(A)\}$ denote a state localized within A . Then, for each incomplete momentum P on T^*M , there exist (infinitely) many complete momenta P_α such that the action of the globally well-defined operator $Q(P_\alpha)$ on a localized state ψ is given by

$$Q(P_\alpha)\psi = Q_0(P)\psi ;$$

so that every $Q(P_\alpha)$ may be interpreted as a globally defined observable locally equivalent to P .

- [51] A momentum P defined over a complete Riemannian manifold (M, G) is quantizable if and only if P is globally measurable, both classically and quantum mechanically.

While it is clear that this axiom implies the completeness of a momentum necessary for the application of Mackey's scheme of quantization, the proposed quantizability axiom is nevertheless more restrictive in that at least some complete momenta are not, in the present formulation, quantum globally measurable. However we consider that, in view of the manifest physical origin of the concepts of global measurability, this new axiom is greatly preferable to the purely formal and mathematically engendered constraint of completeness which appears in Mackey's original scheme.

Turning now to the prospect of further work arising from the content of this chapter, and discounting some purely technical questions as yet outstanding in connection with the assimilation into the scheme of momenta "with critical points", we present here a summary programme of the medium term goals of such research which affords a prospect of the potential inherent in the ideas of classical and quantum global measurability. The programme comprises;

- [52] the explicit determination of the class of classically globally measurable momenta, and of the class of quantum globally measurable momenta, so as in particular to determine whether (as we at present conjecture) a momentum is classically globally measurable if and only if it is complete,

- [53] the explicit determination of the class of exactly classically globally measurable momenta, so as to discover whether and of what character are any such non-Killing momenta, and

[54] an exploration of possible alternative formulations of the physical idea of quantum (and if necessary classical) global measurability, so as to enlarge the class of so measurable momenta, and in particular to discover whether the class of quantum globally measurable momenta can be so chosen as to coincide both with the set of classically globally measurable momenta and with the class of complete momentum observables.

The kernel idea of this proposed research consists in the physical content of the axiom of quantizability [51], and its attempted reconciliation with the scheme of Mackey.

In conclusion we may observe that the universality of the measuring process demand for a full comparison of theory with experiment has resulted in the selection of certain global and geometrical properties of the momentum and the space. It is striking that these properties are so strongly related to the conditions required of a momentum and the free Hamiltonian in the purely abstract problem of their quantization.

References to Chapter 1

References to Chapter 1

- 1: Mackey G.W.: "The Mathematical Foundations of Quantum Mechanics",
W.A. Benjamin (1963), §1.3, §2.6.
- 2: Hermann R.: "Yang Mills, Kaluza-Klein, and the Einstein Programme",
Math. Sci. Press (1978), pp 88-92.
- 3: Varadarajan V.S.: "Geometry of Quantum Theory", volume 2, Van
Nostrand Reinhold (1970), p 148.
- 4: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978), §5.4, pp 425-439.
- 5: Loomis L.H. and Sternberg S.: "Advanced Calculus", Addison-Wesley
(1968), Chapter 13, pp 509-567.
- 6: Guest P.B.: "The Quantization of Classical Systems", Rep. Math.
Phys. 6 99-157.
- 7: Loomis L.H. and Sternberg S.: "Advanced Calculus", Addison-Wesley
(1968), Chapter 10, §5, §6 pp 416-427.
- 8: Mackey G.W.: "The Mathematical Foundations of Quantum Mechanics",
W.A. Benjamin (1963), §1.3, §2.6.
- 9: Varadarajan V.S.: "Geometry of Quantum Theory", volume 2, Van
Nostrand Reinhold (1970), p 148.
- 10: Hermann R.: "Yang-Mills, Kaluza-Klein, and the Einstein Programme",
Math. Sci. Press (1978) p 92.
- 11: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978), p 141 proposition 2.6.14.
- 12: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant
Curvature", Prog. Theor. Phys. 58 (1977) 1030-
- 13: Brickell F. and Clark R.S.: "Differentiable Manifolds", Van
Nostrand Reinhold (1970) p 140, proposition 8.3.2.
- 14: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978) p 142 proposition 2.6.15.

- 15: Capri A.Z.: "Self-Adjointness and Spontaneously Broken Symmetry",
Am. J. Phys. 45 (1977) 823-
- 16: Dicke R.H. and Wittke J.P.: "Introduction to Quantum Mechanics",
Addison-Wesley (1963) p 54.
- 17: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant
Curvature", Prog. Theor. Phys. 58 (1977) 1030-
- 18: Courant R. and Hilbert D.: "Partial Differential Equations",
volume 2, Interscience (1962) p 622.
- 19: Aharanov Y. and Safko J.L.: "Measurement of Noncanonical Variables",
Ann. Phys. 91 (1975), 279.
- 20: Eisenhart L.P.: "Riemannian Geometry", Princeton (1926) pp 3-5.
- 21: Synge J.L.: "Relativity, the General Theory", North Holland (1971),
§2.2, §2.3.
- 22: Synge J.L. and Schild A.: "Tensor Calculus", University of Toronto
Press (1966), §2.6 pp 58-72.
- 23: Kreyszig E.: "Introductory Mathematical Statistics", Wiley (1970),
§6.2 pp 79-80.
- 24: Kreyszig E.: "Introductory Mathematical Statistics", Wiley (1970),
§17.1 pp 319-321.
- 25: Akhiezer N.I. and Glasman I.M.: "Theory of Linear Operators in
Hilbert Space", volume 1, Frederick Ungar (1961), p 110.
- 26: Roman P: "Advanced Quantum Theory", Addison-Wesley (1965), §1.4
p 30.
- 27: Britten W.E. ed.: "Lectures in Theoretical Physics", volume VIII A,
Gordon and Breach (1966) pp 1-64, p 15.
- 28: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978) p 431.
- 29: Chernoff P.: "Essential Self-Adjointness of powers of generators of
hyperbolic equations", J. Funct. Anal. 12 (1973) 401-414.
- 30: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978) exercise 3.3E p 200.

Appendices to Chapter 1

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Appendix 1: On Mackey's Scheme of Quantization.

We give in this section an indication of the constructional steps involved in the quantization scheme for the complete momenta proposed firstly by G.W. Mackey. We shall in the foregoing sections follow closely the notational conventions and terminology of Loomis and Sternberg^(al).

- [1] The identification of the one-parameter group of transformations of M , $\{\Phi_t | t \in \mathbb{R}\}$.

For a complete momentum P the associated C^∞ vector field X over M has a flow $\phi: M \times \mathbb{R} \rightarrow M$ satisfying the following conditions;

$$\forall x \in M, \forall t, s \in \mathbb{R}, \phi(x, 0) = x, \phi(\phi(x, s), t) = \phi(x, s+t), \quad (A1.1)$$

from which it is immediate that the maps $\Phi_t: M \rightarrow M$ defined by $\Phi_t(x) = \phi(x, t)$ constitute a one-parameter group of transformations of M .

- [2] Construction of a one-parameter group of unitary transformations $\{U_t | t \in \mathbb{R}\}$ of $\mathcal{L}^2_\rho(M)$ naturally induced by $\{\Phi_t | t \in \mathbb{R}\}$.

We simply demonstrate that the maps $U_t: \mathcal{L}^2_\rho(M) \rightarrow \mathcal{L}^2_\rho(M)$ defined by

$$U_t \psi = (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* \psi, \quad (A1.2)$$

form such a one-parameter group. The proof proceeds by several steps.

Lemma 1.1: The symbolic form $(\Phi_t^* \rho / \rho)^{\frac{1}{2}}$ defines a function on M .

proof: Let (U_α, α) and (U_β, β) , $U_\alpha \cap U_\beta \neq \emptyset$ denote two charts of some atlas of M ; then, since $\Phi_t^* \rho$ and ρ are both C^∞ densities on M , we have that by definition,

$$(\Phi_t^* \rho)_\alpha(\alpha(x)) = (\Phi_t^* \rho)_\beta(\beta(x)) |\det J_{\beta \circ \alpha^{-1}}|, \quad (A1.3)$$

$$(\rho)_\alpha(\alpha(x)) = (\rho)_\beta(\beta(x)) |\det J_{\beta \circ \alpha^{-1}}|, \quad (A1.4)$$

where $J_{\beta\circ\alpha^{-1}}$ is the Jacobian matrix characterising the transformation between the coordinates α and β , and is given in terms of the component coordinate maps α^i, β^j by $(\partial\beta^j/\partial\alpha^i)$. Hence defining the quotient $\Phi_t^*\rho/\rho$ within each chart (U_α, α) by the prescription,

$$(\Phi_t^*\rho/\rho)_\alpha(\alpha(x)) = (\Phi_t^*\rho)_\alpha(\alpha(x))/(\rho)_\alpha(\alpha(x)) , \quad (A1.5)$$

we immediately perceive that the structure $\Phi_t^*\rho/\rho$ transforms as a function on $\mathcal{L}_\rho^2(M)$. Moreover, since $\rho > 0$, and since by definition and for a suitably chosen chart (U_β, β) ,

$$(\Phi_t^*\rho)_\alpha(\alpha(x)) = |\det J_{\beta\circ\Phi_t\circ\alpha^{-1}}| (\rho)_\beta(\beta\circ\Phi_t\circ\alpha^{-1}(\alpha(x))) , \quad (A1.6)$$

$\Phi_t^*\rho > 0$, we perceive that the quotient $(\Phi_t^*\rho)_\alpha(\alpha(x))/(\rho)_\alpha(\alpha(x))$ is both differentiable and strictly positive, and hence that the square root $(\Phi_t^*\rho/\rho)^{\frac{1}{2}}$ is globally well-defined.

Lemma 1.2: U_t has unitary action on $\mathcal{L}_\rho^2(M)$.

proof: We have that $\forall \phi, \psi \in \mathcal{L}_\rho^2(M)$

$$(U_t\psi, U_t\phi) = \int_M \overline{(U_t\psi)} U_t\phi \rho = \int_M \Phi_t^*(\bar{\psi}\phi\rho) ; \quad (A1.7)$$

hence, observing that Φ_t is a diffeomorphism on M , we deduce^(a2)

$$\int_M \Phi_t^*(\bar{\psi}\phi\rho) = \int_M \bar{\psi}\phi\rho = (\psi, \phi) , \quad (A1.8)$$

which completes the proof.

Theorem 1.3: The set of maps $\{U_t | t \in \mathcal{R}\}$ forms a one-parameter group of transformations of $\mathcal{L}_\rho^2(M)$.

proof: It suffices to show that $\forall t, s \in \mathcal{R}, U_t \circ U_s = U_{t+s}$. We have

$$\begin{aligned}
U_t \circ U_s &= (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* [(\Phi_s^* \rho / \rho)^{\frac{1}{2}} \Phi_s^*] \\
&= ((\Phi_t^* \circ \Phi_s^*) \rho / \rho)^{\frac{1}{2}} (\Phi_t^* \circ \Phi_s^*) = (\Phi_{t+s}^* \rho / \rho)^{\frac{1}{2}} \Phi_{t+s}^* = U_{t+s},
\end{aligned}
\tag{A1.9}$$

since it is readily demonstrated that $\Phi_t^* (\Phi_s^* \rho / \rho) = (\Phi_t^* \circ \Phi_s^* \rho) / (\Phi_t^* \rho)$, by appeal to the coordinate-based definition of $\Phi_t^* \rho / \rho$.

[3] Identification of the unique self-adjoint operator Ω such that

$$\forall t \in \mathbb{R} \quad U_t = \exp(-i\Omega t / \hbar) . \tag{A1.10}$$

We remark simply that the existence of such a Ω is an immediate consequence of Stone's theorem^(a3); the exact form of Ω will be discussed in appendix 2.

[4] Prescription of an essentially self-adjoint operator whose closure may be identified with $Q(P) = \Omega$.

We first demonstrate that Ω , when restricted to the dense subset $C_0^\infty(M)$ of $\mathcal{L}_\rho^2(M)$, assumes the form,

$$Q_0(P) = -i\hbar(X + \frac{1}{2} \operatorname{div} X) , \tag{A1.11}$$

it being immediate that $Q_0(P)$ on $C_0^\infty(M)$ is symmetric. We need only prove that

$$\forall \psi \in C_0^\infty(M) \quad Q_0(P)\psi = \lim_{t \rightarrow 0} \frac{U_t \psi - \psi}{t} . \tag{A1.12}$$

We argue as follows:

$$\begin{aligned}
&\lim_{t \rightarrow 0} [(\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* \psi - \psi] t^{-1} \\
&= \lim_{t \rightarrow 0} [(\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* \psi - (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \psi] t^{-1} + \lim_{t \rightarrow 0} [(\Phi_t^* \rho / \rho)^{\frac{1}{2}} \psi - \psi] t^{-1} \\
&= X\psi + \frac{1}{2} \rho^{-1} \psi \lim_{t \rightarrow 0} [\Phi_t^* \rho - \rho] t^{-1} = X\psi + \frac{1}{2} \operatorname{div} X \psi ,
\end{aligned}
\tag{A1.13}$$

where we have observed that all the limits exist and hence justify the above decomposition a posteriori. Finally we demonstrate that the above defined operator $Q_0(P)$ is essentially self-adjoint, to which end we state the following lemma.

Lemma 1.4: Let Ω be an (unbounded) self-adjoint operator on a Hilbert space H ; let D_0 , a subset of the domain of Ω , be a dense linear subspace of H , and suppose that $U_t = \exp i\Omega t$, the unitary one-parameter group associated with Ω , leaves D_0 invariant. Then the restriction Ω_0 of Ω to D_0 is essentially self-adjoint.

Proof: see Abraham and Marsden^(a4).

We may now state and prove this last result.

Theorem 1.5: On the essential self-adjointness of $Q_0(P)$.

The operator $Q_0(P)$ as defined above on $C_0^\infty(M)$ is essentially self-adjoint.

Proof: We demonstrate in accordance with lemma 1.4 that

$$\forall t \in \mathbb{R} \quad U_t C_0^\infty(M) = C_0^\infty(M) . \quad (A1.14)$$

For let $\psi \in C_0^\infty(M)$, then $U_t \psi = (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* \psi \in C_0^\infty(M)$, and if $U_t \psi \in C_0^\infty(M)$, then $\psi = U_{-t}(U_t \psi) \in C_0^\infty(M)$, and the result follows.

Appendix 2: The Explicit Representation of a Complete Quantum Momentum.

Since $Q_0(P)$ is, by hypothesis of theorem 2 of chapter 1, essentially self-adjoint, to determine the self-adjoint extension $Q(P) = Q_0^\dagger(P)$ of $Q_0(P)$ we need only obtain the adjoint of any symmetric extension of $Q_0(P)$. We therefore state and prove the following theorem.

Theorem 2.1: The Adjoint $Q_1^\dagger(P)$ of $Q_1(P)$.

The operator $Q_1(P)$ defined over the Hilbert space $\mathcal{L}_\rho^2(M)$ of a Riemannian manifold M by the differential expression

$$Q_1(P) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) , \quad (\text{A2.1})$$

on the domain

$$DQ_1(P) = \{ \psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C_0^1(X, M), Q_1(P)\psi \in \mathcal{L}_\rho^2(M) \} , \quad (\text{A2.2})$$

in which $C_0^1(X, M)$ denotes the class of $C^1(X, M)$ functions of compact support, has the adjoint $Q_1^\dagger(P)$ given explicitly by

$$Q_1^\dagger(P) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) , \quad (\text{A2.3})$$

on the domain

$$DQ_1^\dagger(P) = \{ \psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X, M), Q_1^\dagger(P)\psi \in \mathcal{L}_\rho^2(M) \} . \quad (\text{A2.4})$$

Proof: Define the operator Ω by the differential expression

$$\Omega = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) , \quad (\text{A2.5})$$

and domain

$$D\Omega = \{ \psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X, M), \Omega\psi \in \mathcal{L}_\rho^2(M) \} . \quad (\text{A2.6})$$

We demonstrate that $Q_1^\dagger(P) = \Omega$ by showing first that $\Omega \subseteq Q_1^\dagger(P)$, and then that $Q_1^\dagger(P) \subseteq \Omega$.

[1] Ω is a restriction of $Q_1^\dagger(P)$.

We show explicitly that

$$\forall \psi \in D\Omega, \forall \phi \in DQ_1(P) \quad (\psi, Q_1(P)\phi) = (\Omega\psi, \phi) . \quad (A2.7)$$

For we have that

$$\begin{aligned} (\psi, Q_1(P)\phi) &= -i\hbar \lim_{t \rightarrow 0} [(\psi, \Phi_t^* \phi) - (\psi, \phi)] t^{-1} - \frac{i\hbar}{2} (\psi, \operatorname{div} X\phi) \\ &= -i\hbar \lim_{t \rightarrow 0} \int_M \Phi_t^* (\phi \Phi_{-t}^* (\bar{\psi}\rho)) - (\psi, \phi)] t^{-1} - \frac{i\hbar}{2} (\psi, \operatorname{div} X\phi) . \end{aligned} \quad (A2.8)$$

Now, observing that the density $\phi \Phi_{-t}^* (\bar{\psi}\rho)$ is of compact support we have

$$\begin{aligned} (\psi, Q_1(P)\phi) &= -i\hbar \lim_{t \rightarrow 0} \int_M \phi \Phi_{-t}^* (\bar{\psi}\rho) - (\psi, \phi)] t^{-1} - \frac{i\hbar}{2} (\psi \operatorname{div} X, \phi) \\ &= i\hbar \int_M \phi D_X (\bar{\psi}\rho) - \frac{i\hbar}{2} (\operatorname{div} X\psi, \phi) = (\Omega\psi, \phi) . \end{aligned} \quad (A2.9)$$

It is now immediate that $\Omega \subseteq Q_1^\dagger(P)$ and that, since $D\Omega \supset DQ_1(P)$ that $Q_1(P)$ is indeed symmetric.

[2] $Q_1^\dagger(P)$ is a restriction of Ω .

The proof of this result lies in the observation that if a family $\{A_\alpha\}$ of finite¹ and simply connected sets A_α exists in M such that $\bigcup_\alpha A_\alpha$ includes almost every point of M , and if the system of equations

$$\forall \phi \in \bigcup_\alpha C_O^1(X, A_\alpha) \quad (\psi, Q_1(P)\phi) = (\psi^\dagger, \phi) \quad (A2.10)$$

define, for all ψ in the domain $D\Sigma$, a function ψ^\dagger almost everywhere in M ; then the operator Σ defined by the prescription $\forall \psi \in D\Sigma, \Sigma\psi = \psi^\dagger$ is an extension of the adjoint $Q_1^\dagger(P)$, since $DQ_1(P) \supset \bigcup_\alpha C_O^1(X, A_\alpha)$.

¹ Here finite is taken to mean having non-zero but finite measure.

It will be sufficient therefore to demonstrate that $\Omega = \Sigma$ with a suitable choice of the family of sets $\{A_\alpha\}$.

Lemma 2.2: The sets A_α may be indexed by the points $x \in M$ as follows:

- (i) If $x \in M$: $X(x) \neq 0$ then there exists a finite and simply connected region $A_x \ni x$ around x upon which there exists a local canonical coordinate system $\{x^i | i \in [1, n]\}$ in which $X = \partial/\partial x^1$.
- (ii) If $x \in M$: $X(x) = 0$ then either
 - (a) x is an interior point of the set $K = \{x \in M | X(x) = 0\}$ of critical points, when we elect a finite and simply connected set $A_x \subset K$, or else
 - (b) x is on the boundary ∂K of K , when no convenient set A_x can be constructed. However in this latter case the set ∂K is of measure zero.

note: that the set ∂K contains all the isolated critical points of X .

proof: (i) Brickell and Clark^(a5), (ii) clear.

Lemma 2.3: The system of integral equations,

$$\forall \phi \in C_0^1(X, A_x) \quad \int_{A_x} \psi^* \rho D_X \phi = 0 \quad (A2.11)$$

is satisfied if and only if

$$D_X(\psi \rho) = 0 \quad (A2.12)$$

almost everywhere in A_x .

proof: if: Suppose $D_X(\psi \rho) = 0$ almost everywhere on A , then we have

$$\int_{A_X} D_X(\psi^* \phi \rho) = \int_{\partial A_X} \psi^* \phi \epsilon_X \rho_X = 0, \quad (A2.13)$$

by the divergence theorem, and moreover

$$\int_{A_X} D_X(\psi^* \phi \rho) = \int_{A_X} D_X(\psi^* \rho) \phi + \int_{A_X} \psi^* \rho D_X \phi = 0, \quad (A2.14)$$

whence immediately the result.

only if: If $A_X: X(x) = 0$ then the result is trivial.

Otherwise $A_X: X(x) \neq 0$ and the equation (A2.11)

expressed in terms of the local canonical coordinates

$\{x^i | i \in [1, n]\}$ becomes

$$\forall \phi \in C^1_0(X, A_X) \quad \int_{A_X} \psi^* \frac{\partial \phi}{\partial x^1} \sqrt{g} \, dx^1 \dots dx^n = 0. \quad (A2.15)$$

This equation may now be regarded as an equation in

the Hilbert space $L^2_\rho(A_X)$, when plainly ψ must lie in

the domain of the adjoint of $\frac{\partial}{\partial x^1}$. A simple extension

of the result of Wan & Viazminsky^(a6) then shows that

$\psi \in C^1(X, A_\alpha)$. Hence from the identity

$$\int_{A_X} D_X(\phi \psi^* \rho) = 0 = \int_{A_X} D_X(\psi^* \rho) \phi + \int_{A_X} \psi^* \rho D_X \phi, \quad (A2.16)$$

we deduce that $D_X(\psi^* \rho) = 0$ and therefore that

$D_X(\psi \rho) = 0$ as required.

Lemma 2.4: For every set A_X of the above defined family

$\{A_X | x \in M - \partial K\}$ we have that the system of equations

$$\forall \phi \in C^1_0(X, A_\alpha) \quad (\psi, Q_1(P)\phi) = (\psi^\dagger, \phi) \quad (A2.17)$$

requires that $\psi \in C^1(X, A_X)$ and that

$$\psi^\dagger(y) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X)\psi(y) \quad \forall y \in A_X \quad (A2.18)$$

proof: Suppose initially that $X(x) \neq 0$, and introduce the

locally defined functions ξ and η by

$$\operatorname{div}(\xi X) = D_X(S\rho)/\rho = \psi^\dagger, \quad \operatorname{div}(\eta X) = D_X(\eta\rho)/\rho = \frac{1}{2}i\hbar\psi \operatorname{div} X. \quad (\text{A2.19})$$

These functions are $C^1(X, A_X)$ and have the coordinate representations, in terms of the local canonical chart,

$$\xi(x^k) = g^{-\frac{1}{2}} \int x^1 \psi^\dagger \sqrt{g} \, dx^1 + \xi_0(x^2 \dots x^n) g^{-\frac{1}{2}}, \quad (\text{A2.20})$$

$$\eta(x^k) = \frac{1}{2}i\hbar g^{-\frac{1}{2}} \int x^1 \psi \operatorname{div} X \sqrt{g} \, dx^1 + \eta_0(x^2 \dots x^n) g^{-\frac{1}{2}}, \quad (\text{A2.21})$$

in which the functions η_0, ξ_0 are arbitrary functions, and give rise, together with the divergence theorem, to the identities

$$\int_M D_X(\phi * \xi \rho) = (\phi, \operatorname{div}(\xi X)) + (D_X \phi, \xi) = 0, \text{ and} \quad (\text{A2.22})$$

$$\int_M D_X(\phi * \eta \rho) = (\phi, \operatorname{div}(\eta X)) + (D_X \phi, \eta) = 0. \quad (\text{A2.23})$$

Substituting the expressions (A2.22), (A2.23) into the system (A2.17) we deduce that

$$\forall \phi \in C_O^1(X, A_X) \quad \int_{A_X} (i\hbar\psi + \xi - \eta) (D_X \phi)^* \rho = 0. \quad (\text{A2.24})$$

But now this result implies, by lemma 2.3 above, that

$$\rho(i\hbar\psi + \xi - \eta) = \rho_0, \quad \text{where } D_X \rho_0 = 0 \quad (\text{A2.25})$$

so that we have immediately that $\psi \in C^1(X, A_X)$.

Applying the operator $\rho^{-1} D_X$ to (A2.25), and substituting from (A2.19), we deduce

$$\psi^\dagger = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X)\psi \quad \forall y \in A_X. \quad (\text{A2.26})$$

Suppose finally that $X(x) = 0 \quad x \notin \partial K$, then $\operatorname{div} X = 0$ almost everywhere in A_X so that (A2.11) becomes

$$\forall \phi \in C_O^1(X, A_X) \quad (\psi^\dagger, \phi) = 0, \quad (\text{A2.27})$$

which implies directly that $\psi^\dagger = \operatorname{div} X \psi = 0$ and this being

$$\text{true } \forall \psi \in \mathcal{L}_\rho^2(A_X) = C^1(X, A_X).$$

This completes the proof of the proposition.

Theorem 2.4: The operator defined by the equations

$$\forall \phi \in \bigcup_X C_O^1(X, A_X) \quad \forall \psi \in D\Sigma \quad (\psi, Q_1(P)\phi) = (\Sigma\psi, \phi) \quad (\text{A2.28})$$

is equal to Ω .

proof: We have by lemma 2.4 that for every A_X

$$\forall \psi \in C^1(X, A_X) \quad \forall y \in A_X \quad (\Sigma\psi)(y) = (\Omega\psi)(y), \quad (\text{A2.29})$$

and hence, combining this result for all the sets A_X we deduce

$$\forall \psi \in \bigcap_X C^1(X, A_X) = C^1(X, M) \quad \forall y \in M - \partial K \quad (\Sigma\psi)(y) = (\Omega\psi)(y). \quad (\text{A2.30})$$

Thus finally, noting that the functions $\Sigma\psi$ must be square-integrable on M , we obtain

$$\Sigma\psi = -i\hbar(D_X + \frac{1}{2} \text{div } X). \quad (\text{A2.31})$$

$$D\Sigma = \{\psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X, M), \Sigma\psi \in \mathcal{L}_\rho^2(M)\}, \quad (\text{A2.32})$$

which is the desired result.

This completes the demonstration of the grand Theorem 2.1.

Appendix 3: On the Dequantization of a Quantum Momentum.

[1] The inverse of Mackey's theorem for a one-dimensional manifold.

It will be sufficient to consider an "interval" manifold $M = (a, b)$, $a, b \in \overline{\mathbb{R}}^1$; for if M were homeomorphic to a circle S^1 , then, since S^1 is compact, all the vector fields of M would be complete^(a7). We will, restricting our attention to these momenta where associated vector fields X have no critical points, simply state and prove the required result.

Theorem 3.1: Let P be a momentum generating a C^∞ vector field $X = \xi(x) \frac{d}{dx}$, $\xi(x) \neq 0$, on the Riemannian manifold $(M, G) = ((a, b), g_{11}(x))$, $a, b \in \overline{\mathbb{R}}$, and let the self-adjoint operator Ω on $\mathcal{L}^2_{\sqrt{g}}(a, b)$ possess a symmetric restriction Ω_0 of the form

$$\Omega_0 = -i\hbar \left(\xi(x) \frac{d}{dx} + \frac{1}{2\sqrt{g}} \frac{d}{dx} (\xi\sqrt{g}) \right), \quad (\text{A3.1})$$

on a domain

$$D\Omega_0 = \{ \psi \in \mathcal{L}^2_{\sqrt{g}}(a, b) \mid \psi \in C^\infty_0(a, b), \Omega_0 \psi \in \mathcal{L}^2_{\sqrt{g}}(a, b) \}. \quad (\text{A3.2})$$

Then the momentum P and the vector field X are complete only if Ω_0 is essentially self-adjoint.

Proof: The proof is based upon an application of the following lemma.

Lemma 3.2: A symmetric operator Ω_0 is essentially self-adjoint if and only if its adjoint Ω_0^\dagger has no eigenfunctions corresponding to $\pm i$.

proof: Suppose first that Ω_0 is essentially self-adjoint, that is that the sets $(\Omega_0 \pm iE)D\Omega_0$, where E denotes the identity operator, are dense^(a8) in the Hilbert space H . We then have that

¹ $\overline{\mathbb{R}}$ denotes the extended real numbers $\mathbb{R} \cup \{-\infty, +\infty\}$.

$$\forall \psi \in D\Omega_0^\dagger, \forall \phi \in D\Omega_0, (\Omega_0^\dagger \pm iE)\psi = 0 \Rightarrow \langle \psi | \Omega_0 \pm iE \phi \rangle = 0, \quad (\text{A3.3})$$

and hence, since $(\Omega_0 \pm iE)\phi$ is dense in H , that $\psi = 0$.

Next assume that $(\Omega_0^\dagger \pm iE)\psi = 0 \Rightarrow \psi = 0$, and consider the set $[(\Omega_0 \pm iE)D\Omega_0]^\perp$, the perpendicular complement of $(\Omega_0 \pm iE)D\Omega_0$; then we have that

$$\forall \psi \in [(\Omega_0 \pm iE)D\Omega_0]^\perp, \forall \phi \in D\Omega_0 \quad \langle (\Omega_0 \pm iE)\phi | \psi \rangle = 0, \quad (\text{A3.4})$$

so that $\psi \in D\Omega_0^\dagger$, and that therefore, because $D\Omega_0$ is dense in H ,

$$\langle \phi | (\Omega_0^\dagger \pm iE) | \psi \rangle = 0 \Rightarrow (\Omega_0^\dagger \pm iE)\psi = 0. \quad (\text{A3.5})$$

But this last equation requires, by hypothesis, that $\psi = 0$, so that we have shown that $(\Omega_0 \pm iE)D\Omega_0$ is dense in H .

The adjoint Ω_0^\dagger of the operator Ω_0 above, required for the utilisation of lemma 3.2, is given explicitly by

Lemma 3.3: The adjoint Ω_0^\dagger is defined explicitly by

$$\Omega_0^\dagger = -i\hbar(\xi(x) \frac{d}{dx} + \frac{1}{2\sqrt{g}} \frac{d}{dx} (\xi\sqrt{g})) , \quad (\text{A3.6})$$

on the domain

$$D\Omega_0^\dagger = \{ \psi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \mid \psi \in C^1(a,b), \Omega_0^\dagger \psi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \} . \quad (\text{A3.7})$$

proof: see Wan and Viazminsky^(a9) for a complete proof: otherwise observe that $\Omega_0 = Q_0(P) \subset Q_1(P)$ as defined in appendix 2, so that $\Omega_0^\dagger \supseteq Q_1^\dagger(P)$, and that therefore Ω_0^\dagger contains the domain (A3.7) upon which it acts with the differential expression (A3.6).

We next determine the formal "eigenfunctions" of the operator Ω_0^\dagger which correspond to $\pm i$, and obtain the expressions

$$\psi_{i\mu}(x) = \alpha_{\mu} (\xi\sqrt{g})^{-\frac{1}{2}} \exp\left(\frac{\mu}{\hbar} \int_{x_0}^x \xi^{-1} dx\right), \quad (\text{A3.8})$$

in which $x, x_0 \in (a,b)$, and $\mu \in \{-1,1\}$.

Introducing now the parametrisation of (a,b) defined by the mapping

$t(x) = \int_{x_0}^x \xi^{-1} dx$, we deduce that the normalisation integrals for $\psi_{i\mu}(x)$ become simply

$$\langle \psi_{i\mu} | \psi_{i\mu} \rangle = \int_a^b |\alpha_{\mu}|^2 (\xi\sqrt{g})^{-1} \exp\left(\frac{2\mu}{\hbar} t(x)\right) \sqrt{g} dx = |\alpha_{\mu}|^2 \int_{t(a)}^{t(b)} e^{\frac{2\mu}{\hbar} t} dt. \quad (\text{A3.9})$$

We observe that $\psi_{i\mu}(x) \in C^1(a,b)$, so that $\psi_{i\mu} \in D\Omega_0^+$ if and only if $\psi_{i\mu}(x) \in L^2_{\sqrt{g}}(a,b)$; but now the range of the coordinate $t(x)$ is that of the t -parameter defined on the maximal integral curve of X through $x_0 \in (a,b)$, so that the requirement that X is incomplete (for we prove the theorem in contrapositive form) assumes that one of the following sets of inequalities is satisfied

$$-\infty < t(a) < t(b) < +\infty, \quad -\infty = t(a) < t(b) < +\infty, \quad -\infty < t(a) < t(b) = +\infty. \quad (\text{A3.10})$$

Whichever of these conditions is satisfied, we now observe that at least one of the normalisation integrals $\langle \psi_{i\mu} | \psi_{i\mu} \rangle$ converges, and hence we deduce by lemma 3.2, that Ω_0 is not essentially self-adjoint.

[2] The inverse "Mackey"-problem for an n -dimensional manifold.

In this section we undertake a proof of the result in an n -dimensional manifold. For simplicity we shall retain the assumption that the momentum P has no associated critical points on M . Before stating and proving the principal result we first present some technical considerations in the form of two lemmata.²

Lemma 3.4: Let X be an incomplete C^∞ vector field without critical points on a Riemannian manifold (M,G) . Then there exists an incomplete maximal integral curve $\sigma(t)$ of X starting from some $x_0 \in M$, which satisfies the following.

²The following lemmata and their proofs are intended as illustrations only and may fail in certain cases. This does not, however, affect

- (i) $\sigma(t)$ contains its limit points and is a closed curve.
- (ii) There is an open covering U of $\sigma(t)$ upon which coordinates $\{x^i | i \in [1, n]\}$ exist in which X assumes the form $\partial/\partial x^1$.
- (iii) There exists a C^∞ function $f(x)$ on M such that $\text{supp } f \subset U$ and $f(x) = f(y) \quad \forall x, y \in \sigma(t)$.

proof: (i) Let x_∞ be a limit point of $\sigma(t)$, and let U_∞ be an open neighbourhood of x_∞ in which a canonical coordinate system $\{x^i | i \in [1, n]\}$ exists. Then in terms of this coordinate system x_∞ becomes (x_∞^i) and X becomes $\partial/\partial x^1$, so that the integral curve from x_∞ is represented by the coordinate curve

$$\sigma(t) = (x_\infty^1 + t, x_\infty^2, \dots, x_\infty^n) . \quad (\text{A3.11})$$

Consider now a point $x \in \sigma(t) \cap U_\infty$, which exists since x_∞ is a limit point of $\sigma(t)$. The representation within U_∞ of the integral curve from $x = (x^i)$ is simply

$$\omega(t) = (x^1 + t, x^2, \dots, x^n) ; \quad (\text{A3.12})$$

whence we observe that the representative curves $\sigma(t)$ and $\omega(t)$ in \mathbb{R}^n are parallel curves, and hence either coincide or are disjoint, so that, since x_∞ is a limit point of $\sigma(t)$, it must lie on $\omega(t)$ and hence we have shown that x_∞ lies on $\sigma(t)$. The existence of such a curve, and the fact that it is not closed follow from the observation that every closed integral curve is complete.

- (ii) Introduce a local canonical coordinate chart U_0 of coordinates $\{x^i | i \in [1, n]\}$ around the point $x_0 \in \sigma(t)$,

the validity of theorem 3 of chapter 1 which may be demonstrated by means of the proof sequence of Theorem 2.7 (p.135) upon setting $f = 0$.

such a U_0 existing by theorem^(a7). Observing that the vector field X becomes simply $\partial/\partial x^1$ on U_0 , and that the corresponding flow maps Φ_t become

$$\Phi_t(x^1, \dots, x^n) = (x^1 + t, x^2, \dots, x^n), \quad (\text{A3.13})$$

we may identify the flow parameter t as a function $t(x^1, \dots, x^n)$ defined on U_0 as follows

$$t(x^1, \dots, x^n) \text{ such that } \Phi_t(o, x^2, \dots, x^n) = (x^1, \dots, x^n). \quad (\text{A3.14})$$

We may moreover extend this definition to cover an open neighbourhood U of the curve $\sigma(t)$, provided that no flow lines through U_0 are homeomorphic to a circle, by the following device: Define $t(x)$ implicitly by

$$\forall x \in U \quad x = \Phi_{t(x)}(\alpha(x)), \quad (\text{A3.15})$$

where $\alpha(x) \in U_0$ has the coordinate representation

$$(\alpha^i(x)) = (o, \alpha^2(x), \dots, \alpha^n(x)). \quad (\text{A3.16})$$

Observing that the above also defines the set of functions $\alpha^j(x)$, $j \in [2, n]$, in U , we have only to show that the set of functions $(t, \alpha^2, \dots, \alpha^n)$ form a canonical chart in U covering σ . Along every integral curve of X within U we have $d\alpha^j/dt(x) = 0$, and $dt(x)/dt = 1$, so that indeed $X = \partial/\partial x^1$.

Moreover the coordinates are C^∞ since both the original coordinate maps x^i in U_0 and the maps Φ_t are C^∞ , and thus the proof is complete.

- (iii) Clearly it is possible to elect within U a C^∞ function f , and moreover, we may elect $\text{supp } f \subset U$

so as to contain $\sigma(t)$ ^(a10). Finally observe that $f(x) = f(y) \quad \forall x, y \in \sigma(t)$ is assured by electing $f(x) = f(\alpha^2, \dots, \alpha^n)$ which suffices to define a class of such functions f within U , the global definition of f on M being completed by setting $f(x) = 0 \quad x \notin U$.

Lemma 3.5: The adjoint Ω_0^\dagger of the operator Ω_0 defined by the differential expression

$$\Omega_0 = -i\hbar(X + \frac{1}{2} \operatorname{div} X) , \quad (\text{A3.17})$$

with domain

$$D\Omega_0 = \{\psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C_0^\infty(M), \Omega_0 \psi \in \mathcal{L}_\rho^2(M)\} , \quad (\text{A3.18})$$

has as a restriction the operator

$$\Omega_1^\dagger = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X) , \quad (\text{A3.19})$$

with the domain

$$D\Omega_1^\dagger = \{\psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X, M), \Omega_1^\dagger \psi \in \mathcal{L}_\rho^2(M)\} . \quad (\text{A3.20})$$

proof: This is corollary to the result of appendix 2, where we observe only that $\Omega_1^\dagger = Q_1^\dagger(P)$ and that $Q_1(P) \supset \Omega_0$.

We may now state the principal result of this appendix.

Theorem 3.6: If X is a C^∞ incomplete vector field over a Riemannian manifold (M, G) , then Ω_0 as defined above is not essentially self-adjoint.

Proof: Let $\sigma(t)$ be an incomplete maximal integral curve, and let U be a suitably defined (lemma 3.4) open cover of $\sigma(t)$ within which the canonical coordinate system

$(t, \alpha^2, \dots, \alpha^n)$ exists.

We seek to construct formal eigenfunctions of Ω_0^\dagger corresponding to the eigenvalues $\pm i$ as follows: Introduce (lemma 3.4) a C^∞ function $f(x)$: $\text{supp } f \subset U$ as the arbitrary function determining the eigenfunctions $\psi_{i\mu}(x)$, so that the operator equation defining the $\psi_{i\mu}(x)$ has the form

$$\psi_{i\mu}(x) = 0, \quad x \notin U \quad (\text{A3.21})$$

$$\psi_{i\mu}(x): -i\hbar \left(\frac{\partial}{\partial t} + \frac{1}{2\sqrt{g}} \frac{\partial}{\partial t} \sqrt{g} \right) \psi_{i\mu} = i\mu \psi_{i\mu}, \quad x \in U, \mu \in \{-1, 1\},$$

and results immediately in the formal eigenfunction solutions

$$\psi_{i\mu}(x) = f(x) g^{-\frac{1}{4}} \exp\left(\frac{i\mu}{\hbar} t(x)\right). \quad (\text{A3.22})$$

Observe that, since $f(x) \in C^\infty$ and $\text{supp } f \subset U$, $\psi_{i\mu}(x) \in C^1(X, M)$, and hence that $\psi_{i\mu}(x)$ will lie in $D\Omega_0^\dagger \supseteq D\Omega_1^\dagger$ if and only if $\psi_{i\mu}(x) \in \mathcal{L}_\rho^2(M)$. We consider therefore the scalar products

$$\langle \psi_{i\mu} | \psi_{i\mu} \rangle = \int_U f^2(x) g^{-\frac{1}{2}} \exp\left(\frac{2i\mu}{\hbar} t\right) g^{\frac{1}{2}} dt d\alpha^2 \dots d\alpha^n, \quad (\text{A3.23})$$

so that by Fubini's theorem

$$\langle \psi_{i\mu} | \psi_{i\mu} \rangle = \int f^2(\alpha^2, \dots, \alpha^n) d\alpha^2 \dots d\alpha^n \int_t \exp\left(\frac{2i\mu}{\hbar} t\right) dt. \quad (\text{A3.24})$$

Finally, electing $f(\alpha^2, \dots, \alpha^n)$ such that the "sectional" integral $\int f^2 d\alpha^2 \dots d\alpha^n \neq 0$, we observe that $\langle \psi_{i\mu} | \psi_{i\mu} \rangle$ exists if and only if $\int \exp\left(\frac{2i\mu}{\hbar} t\right) dt$ exists, but now, since $\sigma(t)$ is by hypothesis incomplete, we must have at least one such normalisation integral convergent, and hence by lemma 3.2 we deduce, as required, that Ω_0 is not essentially self-adjoint.

Appendix 4: On the "Complete" Hamiltonians of the Infinite Square-Well.

[1] Theorem 4: A criterion for the "completeness" of the Hamiltonians.

Proof: if: Assume that $(M, G) = ((a, b), \sqrt{g})$ is geodetically complete, and introduce the arc-length parametrisation of (a, b) by $s = \int_{x_0}^x \sqrt{g} dx$, so that the manifold transforms to $(\mathbb{R}, 1)$ and the operator $Q_0(H)$ reduces to the familiar form

$$Q_0(H) = -\frac{\hbar^2}{2m} \frac{d^2}{ds^2}, \quad (A4.1)$$

$$DQ_0(H) = \{\psi \in \mathcal{L}^2(\mathbb{R}) \mid \psi \in C_0^\infty(\mathbb{R}), Q_0(H)\psi \in \mathcal{L}^2(\mathbb{R})\}, \quad (A4.2)$$

which is immediately recognised as essentially self-adjoint in that it has the known^(all) self-adjoint extension

$$Q_0^\dagger(H) = -\frac{\hbar^2}{2m} \frac{d^2}{ds^2}, \quad (A4.3)$$

$$DQ_0^\dagger(H) = \{\psi \in \mathcal{L}^2(\mathbb{R}) \mid \psi \in C^2(\mathbb{R}), Q_0^\dagger(H)\psi \in \mathcal{L}^2(\mathbb{R})\}. \quad (A4.4)$$

only if: Assume that $Q_0(H)$ is essentially self-adjoint, then by lemma 3.2 it has no eigenfunctions corresponding to $\pm i$. Perform as above the transformation to the arc-length parametrisation given by $s = \int_{x_0}^x \sqrt{g} dx$, so that the manifold transforms to $(M, G) = ((s(a), s(b)), 1)$, $s(a), s(b) \in \overline{\mathbb{R}}$, and consider in this representation the eigenfunction equations

$$Q_0^\dagger(H)\psi_{i\mu}(s) = -\frac{\hbar^2}{2m} \frac{d^2}{ds^2} \psi_{i\mu} = i\mu \psi_{i\mu}(s), \quad \mu \in \{-1, 1\}. \quad (A4.5)$$

It is immediate that unless $(s(a), s(b)) = \mathbb{R}$ at least one (non-zero) such solution $\psi_{i\mu}(s) \in DQ_0^\dagger(H)$.

[2] Theorem 5: On the free quantum Hamiltonians.

Proof: The mode of proof is simply to transform the manifold into $(\mathbb{R}, 1)$ and to observe that in the transformed space $Q(H) = Q_0^\dagger(H)$ and $Q(H) = Q^2(P)$, where $Q(P)$ is the momentum of differential expression

$$Q(P) = -i\hbar \frac{d}{ds}, \quad (\text{A4.6})$$

and domain

$$DQ(P) = \{\psi \in \mathcal{L}^2(\mathbb{R}) \mid \psi \in C^1(\mathbb{R}), Q(P)\psi \in \mathcal{L}^2(\mathbb{R})\}. \quad (\text{A4.7})$$

Appendix 5: On the Complete Momenta of the Infinite Square-Well.

[1] Theorem 6: A criterion for the completeness of a momentum.

We first establish the result of theorem 6 for the case of a momentum without critical points on (a,b) as a lemma which will have application in the subsequent proof of the general result.

Lemma 5.1: The statement of theorem 6 is true for the special case of a momentum P without critical points.

proof: Suppose initially that $\xi(x) \frac{d}{dx}$ is complete on (a,b) , and assume, without essential loss of generality, that $\xi(x) > 0$, $x \in (a,b)$; then we may define a coordinate $t(x)$ on (a,b) , which may be identified with the flow-parameter of the vector field, by the equation

$$t(x) = \int_{x_0}^x \frac{dx}{\xi(x)}, \quad x, x_0 \in (a,b). \quad (\text{A5.1})$$

In terms of this coordinate the completeness of the vector field finds expression in the limits

$$\lim_{x \rightarrow a} t(x) = -\infty, \quad \lim_{x \rightarrow b} t(x) = +\infty, \quad (\text{A5.2})$$

so that it is now immediate that

$$\lim_{x \rightarrow a} \xi(x) = \lim_{x \rightarrow b} \xi(x) = 0, \quad (\text{A5.3})$$

and that therefore, since $\xi(x) \in C^\infty[a,b]$,

$$\xi(a) = \xi(b) = 0. \quad (\text{A5.4})$$

Conversely suppose that $\xi(a) = \xi(b) = 0$ and that $\xi(x) \in C^\infty[a,b]$. To demonstrate that $\xi(x)d/dx$ is complete on (a,b) we need only demonstrate that equations (A5.2) are satisfied. Introduce the

Taylor series about the regular point $x = b$

$$\xi(x) = \sum_{K=0}^{\infty} \frac{(-1)^K}{K!} \xi^{(K)}(b) (b-x)^K. \quad (\text{A5.5})$$

Observing that $\xi(x) \neq 0$ $x \in (a,b)$, we perceive that not all the quantities $\xi^{(K)}(b)$ are zero, and that in particular there exists a first such non-zero coefficient, $\xi^{(n)}(b) \neq 0$, say. The generalised mean value theorem then yields

$$\xi(x) = \frac{(-1)^n}{n!} \xi^{(n)}(\eta(x)) (b-x)^n, \quad (\text{A5.6})$$

where $\eta(x) \in (a,b)$. Now $\xi^{(n)}(x) \in C^\infty[a,b]$ is a continuous function, and $(-1)^n \xi^{(n)}(b)$ may be taken, without essential loss of generality, to be positive, so that there exists a range of values $x \in A$ about b in which $\xi^{(n)}(x)$ has the same sign as $\xi^{(n)}(b)$. Thus, defining the set $A = \{x \in [a,b] \mid \text{sign}(\xi^{(n)}(x)) = \text{sign}(\xi^{(n)}(b))\}$, or rather the connected fragment about $x = b$, and the upper bound

$$\xi_0^{(n)} = \sup_{x \in A} [\xi^{(n)}(x) (-1)^n], \quad (\text{A5.7})$$

we deduce the inequalities

$$\lim_{x \rightarrow b} t(x) = \int_{x_0 \in A}^b \frac{dx}{\xi(x)} \geq \int_{x_0}^b \frac{dx}{\xi_0^{(n)} (b-x)^n} \rightarrow +\infty, \quad \forall n \in \mathbb{N}. \quad (\text{A5.8})$$

Thus we have shown that $\lim_{x \rightarrow b} t(x) = +\infty$; an exactly parallel calculation shows that $\lim_{x \rightarrow a} t(x) = -\infty$ and completes the demonstration.

To form the general result for a momentum with critical points we introduce the partition of (a,b) naturally induced by the critical points of the vector field $\xi(x) d/dx$ and given by

$$K_0 = \{x \in (a,b) \mid \xi(x) = 0\}, \quad (\text{A5.9})$$

and the partition of $(a,b) - K_0$ into maximally connected sub-intervals

$$K_n = (a_n, b_n). \quad (\text{A5.10})$$

In the set K_0 the flow map $\Phi_t: (a,b) \rightarrow (a,b)$ become simply $\forall x \in K_0$
 $\forall t \in \mathbb{R} \Phi_t(x) = x$, so that the restriction of $\xi d/dx$ to K_0 is complete.
 Moreover in each set K_n we may, since $\xi(x) \in C^\infty[a_n, b_n]$ and $\xi(a_n) = \xi(b_n) = 0$, apply lemma 5.1 to deduce that $\xi d/dx$ is complete when restricted to each K_n , so that by combining these results we obtain the general result.

note: that provided $\xi(x) \in C^\infty(a,b)$ the conditions $\lim_{x \rightarrow a} \xi(x) = \lim_{x \rightarrow b} \xi(x) = 0$ are necessary ($a, b \in \mathbb{R}$), but not in general sufficient, to assure the completeness of the momentum $\xi(x)p$, as is demonstrated by the counter-example

$$\xi(x) = \sqrt{x}(1-x) \quad \text{on} \quad (M, G) = ((0,1), 1). \quad (\text{A5.11})$$

We need require that $\xi(x)$ be differentiable on the closed interval $[a,b]$.

[2] Theorem 7: On the complete quantum momenta.

The exact form of the differential expression and domain of definition of the complete momentum $Q(\xi(x)p)$ having been given by application of theorem 2 of chapter 1, it remains only to demonstrate that the corresponding spectral function $E(\lambda)$ has the prescribed form. To this end we shall first demonstrate the result in the special case of a momentum without critical points.

Lemma 5.2: The linear momentum on $\mathcal{L}^2(\mathbb{R})$ defined by the differential expression

$$Q(P) = -i\hbar \frac{d}{dx}, \quad (\text{A5.12})$$

on the domain

$$DQ(P) = \{\psi \in \mathcal{L}^2(\mathcal{R}) \mid \psi \in C^1(\mathcal{R}), Q(P)\psi \in \mathcal{L}^2(\mathcal{R})\}, \quad (\text{A5.13})$$

has a spectral function $E(\lambda)$, $\lambda \in \mathcal{R}$, given by

$$E(\lambda)\phi = \int_{-\infty}^{\lambda} \psi(\mu, x) \int_{-\infty}^{+\infty} \phi\psi^*(\mu, x) dx d\mu, \quad (\text{A5.14})$$

in which $\psi(\mu, x)$ is the generalised eigenfunction

$$\psi(\mu, x) = 1/\sqrt{2\pi} \exp \frac{i\mu}{\hbar} x. \quad (\text{A5.15})$$

proof: see Byron & Fuller^(a12).

Lemma 5.3: The spectral function of the operator $O: \mathcal{L}^2_{\sqrt{g}}(a, b) \rightarrow \mathcal{L}^2_{\sqrt{g}}(a, b)$ by $O\psi = 0$, is simply $E(\lambda) = H(\lambda)$, where $H(\lambda)$ is the Heavyside unit-step function^(a13).

proof: $H(-\infty) = 0$, $H(+\infty) = 1$, $H(\lambda_1)H(\lambda_2) = H(\max(\lambda_1, \lambda_2))$,

$$\int_{-\infty}^{+\infty} dH(\lambda) = \int_{-\infty}^{+\infty} \delta(\lambda) d\lambda = 1, \int_{-\infty}^{+\infty} \lambda dH(\lambda) = \int_{-\infty}^{+\infty} \lambda \delta(\lambda) d\lambda = 0.$$

note: the use of Dirac's delta function is inessential, the result following from a rigorous application of the Stieltjes integral^(a14).

Lemma 5.4: The statement of theorem 8 of chapter 1 concerning the spectral function $E(\lambda)$ is correct.

proof: Define the global coordinate $t(x)$ on (a, b) by

$$t(x) = \int_{x_0}^x \xi^{-1}(x) dx, \quad x, x_0 \in (a, b), \text{ in terms of which the proposed spectral function becomes } \forall \phi \in \mathcal{L}^2_{\sqrt{g}}(a, b),$$

$$E(\lambda)\phi = \int_{-\infty}^{\lambda} \psi(\mu, t) \left(\int_{-\infty}^{+\infty} \phi\psi^*(\mu, t) \sqrt{g} \xi dt \right) d\mu, \quad (\text{A5.16})$$

in which

$$\psi(\mu, t) = (2\pi\xi\sqrt{g})^{-\frac{1}{2}} \exp \frac{i\mu}{\hbar} t. \quad (\text{A5.17})$$

Next introduce the auxiliary functions $T(\phi)$ defined by

$$T(\phi) = (\sqrt{g} \xi)^{\frac{1}{2}} \phi, \quad (\text{A5.18})$$

so that $T(\phi) \in \mathcal{L}^2(\mathbb{R})$ if and only if $\phi \in \mathcal{L}^2_{\sqrt{g}}(a,b)$. In terms of these modified functions the function $E(\lambda)\phi$ becomes

$$E(\lambda)\phi = \int_{-\infty}^{\lambda} (\xi\sqrt{g})^{-\frac{1}{2}} T(\psi(\mu, t)) \left(\int_{-\infty}^{+\infty} T(\phi) T(\psi(\mu, t))^* dt \right) d\mu, \quad (\text{A5.19})$$

so that immediately

$$T(E(\lambda)\phi) = \int_{-\infty}^{\lambda} T(\psi(\mu, t)) \left(\int_{-\infty}^{+\infty} T(\phi) T(\psi(\mu, t))^* dt \right) d\mu. \quad (\text{A5.20})$$

We may therefore define a function on $\mathcal{L}^2(\mathbb{R})$ by

$$T(E(\lambda))T(\phi) = T(E(\lambda)\phi), \quad (\text{A5.21})$$

and hence recognise $T(E(\lambda)) = T(\lambda)$ as the known spectral function of lemma 5.2. The spectral properties of $E(\lambda)$ on $\phi \in \mathcal{L}^2_{\sqrt{g}}(a,b)$ are now immediate.

$$\begin{aligned} \text{(i)} \quad T(E(-\infty))T(\phi) &= T(E(-\infty)\phi) = 0 \\ \Rightarrow E(-\infty)\phi &= 0. \end{aligned} \quad (\text{A5.22})$$

$$\text{(ii)} \quad T(+\infty)T(\phi) = T(\phi) \Rightarrow E(+\infty)\phi = \phi. \quad (\text{A5.23})$$

$$\begin{aligned} \text{(iii)} \quad T(\lambda)T(\mu)T(\phi) &= T(\max(\lambda, \mu))T(\phi) \\ \Rightarrow E(\lambda)E(\mu)\phi &= E(\max(\lambda, \mu))\phi. \end{aligned} \quad (\text{A5.24})$$

$$\begin{aligned} \text{(iv)} \quad \int_{-\infty}^{+\infty} dT(\lambda)T(\phi) &= \int_{-\infty}^{+\infty} d(T(E(\lambda)\phi)) = T \int_{-\infty}^{+\infty} dE(\lambda)\phi = T(\phi) \\ \Rightarrow \int_{-\infty}^{+\infty} dE(\lambda)\phi &= \phi. \end{aligned} \quad (\text{A5.25})$$

$$\begin{aligned} \text{(v)} \quad \int_{-\infty}^{+\infty} \lambda dT(\lambda) \cdot T(\phi) &= \int_{-\infty}^{+\infty} \lambda d(T(E(\lambda)\phi)) = T \int_{-\infty}^{+\infty} \lambda dE(\lambda) \cdot \phi \\ &= -i\hbar \frac{d}{dt} (T\phi) \\ \Rightarrow \int_{-\infty}^{+\infty} \lambda dE(\lambda)\phi &= -i\hbar \left(\xi \frac{d}{dx} + \frac{1}{2\sqrt{g}} \frac{d}{dx} (\xi\sqrt{g}) \right) \phi. \end{aligned} \quad (\text{A5.26})$$

Theorem 5.5: The statement of theorem 7 of chapter 1 concerning the spectral function $E(\lambda)$ is true.

proof: Introduce the partition $\{K_n | n \in \mathbb{N}u\{0\}\}$ of the interval (a,b) naturally induced by the critical points of the vector field $\xi(x)d/dx$ and given by

$$K_0 = \{x \in (a,b) | \xi(x) = 0\}, \quad (A5.27)$$

and the partition of $(a,b) - K_0$ into maximally connected subsets K_n by

$$K_n = (a_n, b_n); \quad (A5.28)$$

and observe that, provided K_0 is of non-zero measure, we have that

$$\forall \phi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \quad \chi(K_n)\phi \in \mathcal{L}^2_{\sqrt{g}}(K_n) \quad n \in \mathbb{N}u\{0\}, \quad (A5.29)$$

and that if K_0 is of measure zero then it may be discounted in the following analysis provided only that the proposed spectral operator $E(\lambda)$ when acting on a vector ϕ is assigned a value for every x in K_0 .

We have by lemmata 5.2 and 5.3 that $E(K_n, \lambda)$ obeys the spectral properties (A5.22) - (A5.26) $\forall n \in \mathbb{N}u\{0\}$, $\forall \phi \in \mathcal{L}^2_{\sqrt{g}}(K_n)$, and hence defining the symbolic entity $\chi(K_n)E(K_n, \lambda)$ by

$$\forall \phi \in \mathcal{L}^2_{\sqrt{g}}(a,b) \quad \chi(K_n)E(K_n, \lambda)\phi(x) = \begin{cases} E(K_n, \lambda)\phi(x), & x \in K_n, \\ 0, & x \notin K_n, \end{cases} \quad (A5.30)$$

we deduce by a short calculation that the operator $E(\lambda)$ given by

$$E(\lambda)\phi = \sum_{n \in \mathbb{N}u\{0\}} \chi(K_n)E(K_n, \lambda)\phi, \quad (A5.31)$$

satisfies the desired spectral properties.

Appendix 6: Classical Momentum Measurement in Riemannian Space.

We demonstrate in this appendix the two technical results of §5.2 of chapter 1.

- [1] Given an arbitrary local coordinate system $\{x^i | i \in [1, n]\}$ we may introduce a normal^(a15) coordinate system $\{\bar{x}^i | i \in [1, n]\}$ such that

$$\bar{x}^1 = x^1, \quad g_{ij} dx^i dx^j = \bar{g}_{11} d\bar{x}^1 d\bar{x}^1 + \bar{g}_{\mu\nu} d\bar{x}^\mu d\bar{x}^\nu, \quad \mu, \nu \in [2, n], \quad (\text{A6.1})$$

and hence we may immediately deduce that

$$\bar{p}_1 = (\partial x^i / \partial \bar{x}^1) p_i = p_1. \quad (\text{A6.2})$$

- [2] For a local Cartesian system $\{y^i | i \in [1, n]\}$ we may elect to have y^1 parallel to \bar{x}^1 , so that

$$y^1 = b_1^1 (\bar{x}^1 - a) = b_1^1 (x^1 - a), \quad (\text{A6.3})$$

from which it follows that

$$\bar{p}_1 = (\partial y^i / \partial \bar{x}^1) p_i^0 = b_1^1 p_1^0, \quad b_1^1 = |\bar{g}_{11}|^{\frac{1}{2}} = |g_{11}|^{\frac{1}{2}}. \quad (\text{A6.4})$$

Appendix 7: Measurability and Completeness.

[1] Theorem 9: Standard measurability and completeness.

We state and prove the following result from which theorem 9 is an immediate corollary.

Theorem 7.1: A sphere $S_{d_0}(x) = \{y \in M | d(x,y) = d_0\}$ which is topologically closed may be constructed around every point of a manifold (M,G) if and only if M is geodetically complete.

proof: if: clear.

only if: Let $x \in M$ be any point of M , and construct the local geodesic $\Gamma(x,\alpha)$ through x in a direction α ; then by hypothesis there exists at distance d_0 from x a point y on $\Gamma(x,\alpha)$. Moreover, since y is clearly an interior point of M , we may construct the geodesic $\Gamma(y,\beta)$ such that the fragments $\Gamma(x,\alpha)$, $\Gamma(y,\beta)$ join smoothly at y , and hence we may recursively construct a geodesic $\Gamma(x,\alpha)$ of arbitrary length nd_0 .

[2] Theorem 10: On the properties of an incomplete maximal integral curve on a geodetically complete manifold.

(i) If $\Omega(x_0)$ were a closed curve then $\exists \tau \in \mathcal{R}^+ : \forall t \in (-\tau, \tau) \Phi_t(x) = \Phi_{t+\tau}(x)$ so that the range of t may be extended to \mathcal{R} , thus contradicting our assumption that $\Omega(x_0)$ was incomplete. Equally $\Omega(x_0)$ cannot have end-points, since otherwise it would contradict the known result^(a16) that, at every point of the curve, $\Omega(x_0)$ may be regarded as a coordinate curve.

(ii) We will demonstrate only that

$$\forall \{t_n \geq 0\}_{n \in \mathbb{N}} \xrightarrow{+} \tau^+, \{s(\Omega^+(x_0), x_0, \Phi_{t_n}(x_0))\}_{n \in \mathbb{N}} \xrightarrow{+} +\infty, \quad (\text{A7.1})$$

the analogous result for sequences $\{t_n \leq 0\} \rightarrow \tau^-$ being similarly obtained. Suppose by way of a contradiction that

$$\{s(\Omega^+(x_0), x_0, \Phi_{t_n}(x_0))\} \rightarrow s_0 \in \mathcal{R}; \quad (\text{A7.2})$$

it then follows that

$$\{s(\Omega^+(x_0), x_m, x_n)\}_{n>m} \rightarrow 0 \text{ as } n, m \rightarrow \infty, \quad (\text{A7.3})$$

and hence that

$$\{d(x_m, x_n)\}_{n>m} \rightarrow 0 \text{ as } m, n \rightarrow \infty, \quad (\text{A7.4})$$

since $d(x_m, x_n) \leq s(\Omega^+(x_0), x_m, x_n)$, so that the sequence of points $\{x_n\}_{n \in \mathbb{N}}$ is Cauchy. But since the manifold (M, G) is proper and geodetically complete the Hopf-Rinow^(a17) theorem requires that the sequence $\{x_n\}_{n \in \mathbb{N}}$ converge to a limit x_{τ^+} . Now by lemma 3.4, of appendix 3, $\Omega(x_0)$ contains its limit-points, and x_{τ^+} must be an end-point of $\Omega(x_0)$ which contradicts the statement proved in (i) above. Thus the hypothesis that $s_0 \in \mathcal{R}$ is false and the result required has been demonstrated.

(iii) Simply observe that $R(x_n, \Omega^+(x_n), P) = \tau^+ - t_n \rightarrow 0$ as $t_n \rightarrow \tau^+$.

Appendix 8: On Classical Global Measurability.

Theorem 8.1: Let $\Omega(x_0)$ be an incomplete maximal integral curve of a vector field X without critical points generated by the momentum P , itself defined over a geodetically complete Riemannian manifold (M, G) , and let $\Omega(x_0)$ be such that the range of the t -parametrisation of $\Omega(x_0)$ defined in terms of the flow-maps $\Phi_t: M \rightarrow M$, $\Phi_t(x_0) = x_0$ at $t = 0$, by

$$t(x): \Phi_{t(x)}(x_0) = x, \quad (\text{A8.1})$$

is (τ^-, τ^+) with $\tau^\pm \in \mathbb{R}$. Introduce the arc-length parametrisation of $\Omega(x_0)$ by

$$s(x) = s(\Omega(x_0), x_0, x), \quad s(x) \geq 0 \text{ if and only if } t(x) \geq 0, \quad (\text{A8.2})$$

and let $\{B_n | n \in \mathbb{N}\}$ denote a sequence of local recoil sets B_n along $\Omega(x_0)$ defined by

$$B_n = \{x \in \Omega(x_0) | (n-1)\Delta s \leq s \leq (n+1)\Delta s\}, \quad \Delta s \neq 0. \quad (\text{A8.3})$$

Then the sequence of characteristic local errors $\{\Delta_{B_n} P\}_{n \in \mathbb{N}}$ satisfies

$$\overline{\lim}_{n \rightarrow \infty} \Delta_{B_n} P = +\infty, \quad (\text{A8.4})$$

where $\overline{\lim}$ denotes the limit superior (a18).

note: If $\tau^\pm \notin \mathbb{R}$ the result is valid setting $P \rightarrow -P$ and $X \rightarrow -X$.

Proof: We have by definition that

$$\Delta_{B_n}^2 P = \frac{P^2}{2\Delta s} \int_{(n-1)\Delta s}^{(n+1)\Delta s} (b_1^1(s) - b_1^1(B_n))^2 ds, \quad (\text{A8.5})$$

and that

$$b_1^1(B_n) = \frac{1}{2\Delta s} \int_{(n-1)\Delta s}^{(n+1)\Delta s} b_1^1(s) ds, \quad (\text{A8.6})$$

where clearly $b_1^1(s) \neq 0$, so that we may assume without loss of generality that $b_1^1(s) > 0$. It is now clear that

the problem is intrinsically one-dimensional in character, and we demonstrate the theorem by means of a sequence of technical lemmata, the final result following immediately from lemma 8.7 upon setting $[y_{n-1}, y_{n+1}] = ((n-1)\Delta s, (n+1)\Delta s)$, $y = s$, $\Delta y = \Delta s$, and $\xi(y) = b_1^1(s)$, and upon noting that

$$\int_0^\infty (b_1^1(s))^{-1} ds = \int_0^{\tau^+} (b_1^1(s))^{-1} ds dt = \tau^+ < \infty.$$

Lemma 8.2: A collection of known results.

- (i) Every limit point of a sequence $\{u_n\}$ may be regarded as a limit point of a suitably chosen subsequence $\{u_{n_k}\}$ of $\{u_n\}$.

The convergence of the sum $\sum u_n$ implies that

- (ii) $\lim u_n = 0$;
- (iii) if $u_n > 0$ and $u_{n+1} \leq u_n$, then $\lim n u_n = 0$, and
- (iv) if $u_n > 0$ and $\lim u_n / u_{n+1} = 1$, then $\overline{\lim} n(u_n / u_{n+1} - 1) \geq 1$.
- proof: (i) Knopp^(a19); (ii) Widder^(a20); (iii) Bromwich^(a21);
- (iv) Bromwich^(a22).

Lemma 8.3: Let f_n , the local mean over $[y_n, y_{n+1}]$ of $F(y) > 0$, be defined by

$$f_n \Delta y = f_n (y_{n+1} - y_n) = \int_{y_n}^{y_{n+1}} F(y) dy; \quad (\text{A8.7})$$

then

$$\int_0^\infty F(y) dy < \infty \Rightarrow \underline{\lim} n f_n = 0. \quad (\text{A8.8})$$

proof: Noting the results of lemma 8.2, construct a subsequence of $\{f_n\}$ for which part (iii) holds.

Lemma 8.4: Let \bar{f}_n , the local reciprocal mean, be defined by

$$\bar{f}_n^{-1} = (\Delta y)^{-1} \int_{y_n}^{y_{n+1}} F^{-1}(y) dy ; \quad (\text{A8.9})$$

then

$$\int_0^\infty F(y) dy < \infty \Rightarrow \lim_{n \rightarrow \infty} n \bar{f}_n = 0 . \quad (\text{A8.10})$$

proof: Employ the Schwarz inequality^(a23) to demonstrate that

$\bar{f}_n \leq f_n$, when this proposition is an immediate corollary to lemma 8.3.

Lemma 8.5: Let $\delta_n = \Delta y / (f_{n+1}^{-1} - f_n^{-1})$, where f_n is as above; then $\int_0^\infty F(y) dy < \infty$ implies that $\{\delta_n\}$ has 0 as a limit point. This proposition remains true if f_n is replaced by \bar{f}_n in the statement.

proof: We have

$$\delta_n = \frac{\Delta y \, n f_n}{f_n (n f_n - 1)} , \quad \text{and} \quad \lim_{n \rightarrow \infty} n f_n = 0 . \quad (\text{A8.11})$$

We may distinguish three possible cases:

- (i) $\lim_{n \rightarrow \infty} f_n / f_{n+1} = \alpha \neq 1$, when clearly $\lim_{n \rightarrow \infty} \delta_n = 0$;
- (ii) $\lim_{n \rightarrow \infty} f_n / f_{n+1} = 1$, when we consider a subsequence $\{f_{n_\ell}\}$ of $\{f_n\}$ as selected in the proof of lemma 8.3 and apply lemma 8.2 (iv);
- (iii) f_n / f_{n+1} oscillates indefinitely, when we may construct a suitable subsequence to demonstrate the result.

We now introduce the local standard deviation $\Delta \xi$ of a function $\xi(y)$ on \mathcal{R} over the interval $[a, b]$ defined by

$$(\Delta \xi)^2 = \frac{1}{b-a} \int_a^b (\xi - \bar{\xi})^2 dy , \quad \bar{\xi} = \frac{1}{b-a} \int_a^b \xi dy . \quad (\text{A8.12})$$

We then

Lemma 8.6: We have the inequality

$$(\Delta\xi)^2 \geq \frac{1}{4}(\bar{\xi}_+ - \bar{\xi}_-)^2, \quad (\text{A8.13})$$

$$\text{where } \bar{\xi}_- = \frac{2}{b-a} \int_a^c \xi \, dy, \quad \bar{\xi}_+ = \frac{2}{b-a} \int_c^b \xi \, dy, \quad \text{and } c = \frac{1}{2}(b+a). \quad (\text{A8.14})$$

proof: Introduce $\xi'(y) = \begin{cases} \bar{\xi}_- & , y \in [a, c] \\ \bar{\xi}_+ & , y \in [c, b] \end{cases}$;

$$\text{then deduce by direct calculation } (\Delta\xi'(y))^2 = \frac{1}{4}(\bar{\xi}_+ - \bar{\xi}_-)^2,$$

$$\text{and from the Schwartz inequality } (\Delta\xi)^2 \geq (\Delta\xi')^2.$$

Lemma 8.7: Let $\xi(y) > 0$ be a continuous function on \mathcal{R} , and let

$$(\Delta\xi_n)^2 = \frac{1}{2\Delta y} \int_{y_{n-1}}^{y_{n+1}} (\xi - \bar{\xi}_n)^2 dy, \quad (\text{A8.15})$$

where

$$\bar{\xi}_n = \frac{1}{2\Delta y} \int_{y_{n-1}}^{y_n} \xi \, dy; \quad (\text{A8.16})$$

then

$$\int_0^\infty \frac{dy}{\xi(y)} < \infty \Rightarrow \overline{\lim} \Delta\xi_n = +\infty. \quad (\text{A8.17})$$

proof: We first make the following identifications;

$$\bar{\xi}_n^+ = \frac{1}{\Delta y} \int_{y_n}^{y_{n+1}} \xi(y) \, dy, \quad \bar{\xi}_n^- = \frac{1}{\Delta y} \int_{y_{n-1}}^{y_n} \xi(y) \, dy, \quad (\text{A8.18})$$

$$\bar{f}_n^{-1} = \frac{1}{\Delta y} \int_{y_n}^{y_{n+1}} 1/F(y) \, dy, \quad \bar{f}_{n-1} = \frac{1}{\Delta y} \int_{y_{n-1}}^{y_n} 1/F \, dy,$$

$$F(y) = 1/\xi(y).$$

It then follows that the sequence $\{\bar{\delta}_{n-1}\}$, where

$$\bar{\delta}_{n-1} = \Delta y / (\bar{f}_n^{-1} - \bar{f}_{n-1}^{-1}) = \Delta y / (\bar{\xi}_n^+ - \bar{\xi}_n^-), \quad (\text{A8.19})$$

has 0 as limit point if $\int_0^\infty F(y) dy < \infty$ by lemma 8.5.

It is immediate, therefore, that the sequence $\{\bar{\xi}_n^+ - \bar{\xi}_n^-\}$

has ∞ as a limit point. Finally lemma 8.6 ensures that

$$\int_0^\infty dy/\xi(y) < \infty \Rightarrow \overline{\lim} \Delta\xi_n = +\infty. \quad (\text{A8.20})$$

Appendix 9: On the Existence of Local Momenta.

[1] Theorem 12: On the existence of local momenta.

The proof of this theorem is contained in the sequence of theorems below.

Theorem 9.1: The operator $Q_A^O(P) = \pi Q(P) \pi$, generated by the complete C^∞ momentum P and the projector π onto the set A , is essentially self-adjoint only if A is invariant under the flow of P .

proof: First define the set $C^1(X, A)$ by the prescription

$$C^1(X, A) = \{ \psi \in L^2_\rho(M) \mid D_X \psi(x) \text{ exists } \forall x \in A \} . \quad (A9.1)$$

We may then demonstrate that

$$\forall \phi \in DQ_A^O(P) \quad \forall \psi \in C^1(X, A) \quad \langle \psi \mid Q_A^O(P) \phi \rangle = \langle \psi^\dagger \mid \phi \rangle , \quad (A9.2)$$

where explicitly

$$\psi^\dagger(x) = \begin{cases} -i\hbar(D_X + \frac{1}{2} \operatorname{div} X)\psi(x) , & x \in A , \\ 0 , & x \notin A . \end{cases} \quad (A9.3)$$

For by explicit calculation we obtain the identities;

$$\begin{aligned} (-i\hbar)^{-1} \langle \psi \mid Q_A^O(P) \phi \rangle &= \int_A \bar{\psi} (D_X + \frac{1}{2} \operatorname{div} X) \phi \rho \quad (A9.4) \\ &= \int_A \bar{\psi} (D_X \phi) \rho + \frac{1}{2} \int_A \bar{\psi} \operatorname{div} X \phi \rho \\ &= \lim_{t \rightarrow 0} \left[\int_A \Phi_t^* (\phi \Phi_{-t}^* (\bar{\psi} \rho)) - \int_A \bar{\psi} \phi \rho \right] t^{-1} + \frac{1}{2} \int_A \bar{\psi} \operatorname{div} X \phi \rho \\ &= \lim_{t \rightarrow 0} \left[\int_{\Phi_t(A)} \phi \Phi_{-t}^* (\bar{\psi} \rho) - \int_{\Phi_t(A)} \phi \bar{\psi} \rho \right] t^{-1} + \lim_{t \rightarrow 0} \left[\int_{\Phi_t(A)} \phi \bar{\psi} \rho - \int_A \phi \bar{\psi} \rho \right] t^{-1} \\ &\quad + \frac{1}{2} \int_A \bar{\psi} \operatorname{div} X \phi \rho \\ &= \int_A \phi D_X (\bar{\psi} \rho) + \frac{1}{2} \int_A \phi \operatorname{div} X \bar{\psi} \rho + \int_A D_X (\phi \bar{\psi} \rho) . \end{aligned}$$

Hence, applying the divergence theorem, and substituting the known expression for $\psi^\dagger(x)$, we deduce

$$\langle \psi | Q_A^O(P) \phi \rangle = \langle \psi^\dagger | \phi \rangle - i\hbar \int_{\partial A} \phi \bar{\psi} \epsilon_X^P \quad (A9.5)$$

It remains only to show that the above surface integral vanishes.

Recalling that $\phi \in DQ_A^O(P)$, we must have that $\pi\phi \in C^1(X, M)$, so that we consider the points lying on the boundary ∂A . Let $x \in \partial A$ be any point of ∂A and consider the maximal integral curve $\Omega(x)$ through x . Either $\Omega(x)$ is tangent to ∂A when $\epsilon_X^P(x) = 0$, or else $\Omega(x) = \{x\}$ when x is a critical point of X and $\epsilon_X^P(x) = 0$, or else finally $\Omega(x)$ "cuts" the surface ∂A . Consideration of the definition of $(D_X \pi\phi)$ at x shows that $\pi\phi \in C^1(X, M)$ requires that $\phi(x) = 0$, and therefore that the surface integral of (A9.5) vanishes.

Thus we have shown that $D[Q_A^O(P)]^\dagger$ contains the set $C^1(X, A)$. Further, parallel to the above analysis we have that

$$\forall \phi, \psi \in C^1(X, A) \quad \langle \psi | (Q_A^O(P))^\dagger \phi \rangle = \langle (Q_A^O(P))^\dagger \psi | \phi \rangle - i\hbar \int_{\partial A} \phi \bar{\psi} \epsilon_X^P, \quad (A9.6)$$

and hence the operator $[Q_A^O(P)]^\dagger$ can be symmetric only if

$$\int_{\partial A} \phi \bar{\psi} \epsilon_X^P = 0, \quad (A9.7)$$

or equivalently, as is most readily seen from the fourth line of (A9.4),

$$\Phi_t(A) = A. \quad (A9.8)$$

Finally, therefore, we observe that unless $[Q_A^O(P)]^\dagger$ is symmetric $Q_A^O(P)$ cannot be essentially self-adjoint.

Theorem 9.2: If $\Phi_t(A) = A$, then $Q_A^O(P)$ is essentially self-adjoint, with the self-adjoint extension $Q_A(P) = (Q_A^O(P))^\dagger$ given explicitly by

$$Q_A(P)\psi(x) = \begin{cases} -i\hbar(D_X + \frac{1}{2} \operatorname{div} X)\psi(x) , & x \in A , \\ 0 & , \quad x \notin A , \end{cases} \quad (\text{A9.9})$$

and defined on the domain

$$DQ_A(P) = \{\psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X, A), Q_A(P)\psi \in \mathcal{L}_\rho^2(M)\} . \quad (\text{A9.10})$$

proof: The proof is analogous to that in appendix 2; that the operator $Q_A(P)$ defined by (A9.9) and (A9.10) is a restriction of $[Q_A^O(P)]^\dagger$ follows parallel to the analysis of (A9.4), and that the operator $[Q_A^O(P)]^\dagger$ is a restriction of $Q_A(P)$ can be shown analogously to section [2] of appendix 2.

[2] Theorem 13: On the reconstruction of a global momentum.

We need only observe that

$$\psi \in D(\sum_\alpha Q_{A_\alpha}(P)) = \cap_\alpha DQ_{A_\alpha}(P) \Rightarrow \psi \in C^1(X, M) , \quad (\text{A9.11})$$

and

$$(\forall \alpha \quad Q_{A_\alpha}(P)\psi \in \mathcal{L}_\rho^2(M)) \Rightarrow Q(P)\psi \in \mathcal{L}_\rho^2(M) , \quad (\text{A9.12})$$

so that $Q(P) \subseteq \sum_\alpha Q_{A_\alpha}(P)$.

Similarly we may show that

$$Q(P) \supseteq \sum_\alpha Q_{A_\alpha}(P) ; \quad (\text{A9.13})$$

whence immediately the result.

Appendix 10: On Exact Classical Global Measurability.

[1] Theorem 16: On exact classical global measurability.

If a momentum P is exactly classically globally measurable then, by part [2] below, the function $b_1^1(s) = s_0$, a constant on every integral curve $\Omega(x_0)$ of the associated vector field. Moreover the t -range $R(A, P)$ of any local set over $\Omega(x_0)$ is given by

$$R(A, P) = R(A \cap \Omega(x_0), P) = \int_s^{s+d_0} (b_1^1(s))^{-1} ds = d_0/s_0, \quad (A10.1)$$

as follows from $ds/dt = b_1^1(s)$, and hence it is immediate that P is quantum globally measurable, since d_0 and s_0 are fixed and finite for each integral curve of the vector field.

[2] Theorem 17: On Killing momenta and exact classical global measurability.

If a momentum P is Killing, then in a local chart $\{x^i | i \in [1, n]\}$ the associated vector field $X = \xi^i \frac{\partial}{\partial x^i}$ obeys the differential equations,

$$g_{ij} \xi_{,k}^j + g_{jk} \xi_{,i}^j + g_{ik,j} \xi^j = 0. \quad (A10.2)$$

Introduce in the neighbourhood of any point x in a (non-trivial) maximal integral curve $\Omega(x_0)$ of X the canonical chart $\{t, \alpha^2, \dots, \alpha^n\}$ in terms of which $X = \partial/\partial t$. The Killing equations become simply,

$$\frac{\partial g}{\partial t}{}_{ik} = 0, \quad (A10.3)$$

and hence in particular we have, by (A6.4) that

$$b_1^1(s) = g_{11}^{1/2}(\alpha^2, \dots, \alpha^n) = s_0, \quad (A10.4)$$

is constant on every integral curve of X . It is now immediate that P is exactly classically globally measurable.

note: At least some non-Killing exactly classically globally

measurable momenta must exist since we require only that

$$\partial g_{11}/\partial t = 0 \text{ rather than } \partial g_{ij}/\partial t = 0.$$

[3] Theorem 18: Alternative formulations of exact classical global measurability.

Clearly if $b_1^1(s)$ is constant along every $\Omega(x_0)$ then for every local recoil set B on $\Omega(x_0)$ of whatever length d_0

$$\Delta_B P = 0, \quad (\text{A10.5})$$

and hence P is exactly classically globally measurable.

Equally if $\Delta_B P = 0$ for all local recoil sets B of any length d_0 of every integral curve $\Omega(x_0)$ then

$$\Delta_B P = 0 = \frac{1}{d_0} \int_s^{s+d_0} [b_1^1(s) - b_1^1(B)]^2 ds \quad \forall s \forall d_0 \quad (\text{A10.6})$$

requires that on every integral curve $b_1^1(s) = s_0$, a constant.

The second result that $\partial g_{11}/\partial x^1 = 0$, where $\{x^i | i \in [1, n]\}$ denotes a local canonical coordinate system, follows from the observation

$$(\text{A6.4}) \text{ that } b_1^1(s) = g_{11}^{\frac{1}{2}}(s, x^2, \dots, x^n).$$

References to the Appendices

to

Chapter 1

References to the Appendices
to Chapter 1

- a1: Loomis L.H. and Sternberg S.: "Advanced Calculus", Addison-Wesley (1968), Chapters 9, 10, pp363-428.
- a2: Choquet-Bruhat Y., De Witt-Morette C., and Dillard-Bleick M.: "Analysis, Manifolds and Physics", North Holland (1977), p.205.
- a3: Prugovecki E.: "Quantum Mechanics in Hilbert Space", Academic Press (1971), theorem 6.1, p.335.
- a4: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), lemma 2.6.13, p.141.
- a5: Brickell F. and Clark R.S.: "Differentiable Manifolds", Van Nostrand Reinhold (1970), proposition 8.3.2, p.140.
- a6: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977), 1030-1044.
- a7: Brickell F. and Clark R.S.: "Differentiable Manifolds", Van Nostrand Reinhold (1970), proposition 8.2.6, p.139.
- a8: Hellwig G.: "Differential Operators of Mathematical Physics", Addison-Wesley (1967), definition 1, p.172.
- a9: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977), 1030-1044.
- a10: Matsushima Y.: "Differentiable Manifolds", Van Nostrand Reinhold (1970), lemma 1.2, p.69.
- a11: Kato T.: "Perturbation Theory for Linear Operators", Springer-Verlag (1966), Chapter 5, §5.2.
- a12: Byron Jr. F.W. and Fuller R.W.: "Mathematics of Classical and Quantum Physics", Addison-Wesley (1979), Vol.I, p.283.
- a13: Courant R. and Hilbert D.: "Partial Differential Equations", volume 2, Interscience (1962), p.622.

- a14: Hellwig G.: "Differential Operators of Mathematical Physics", Addison-Wesley (1967), §9.1, pp147-148.
- a15: Synge J.L. and Schild A.: "Tensor Calculus", University of Toronto Press (1966), §2.6, pp58-72.
- a16: Brickell F. and Clark R.S.: "Differentiable Manifolds", Van Nostrand Reinhold (1970), problems 8.1, no.1, p.134; proposition 8.2.2, p.136.
- a17: Choquet-Bruhat Y., De Witt-Morette C., and Dillard-Bleick M.: "Analysis, Manifolds and Physics", North Holland (1977), p.317.
- a18: Knopp K.: "Theory and Applications of Infinite Series", Blackie (1928), §58, pp92-93.
- a19: Knopp K.: "Theory and Applications of Infinite Series", Blackie (1928), p.90.
- a20: Widder D.V.: "Advanced Calculus", Prentice-Hall (1961), p.285.
- a21: Bromwich T.J.I'A.: "An Introduction to the Theory of Infinite Series", MacMillan (1908), p.27.
- a22: Bromwich T.J.I'A.: "An Introduction to the Theory of Infinite Series", MacMillan (1908), p.33.
- a23: Widder D.V.: "Advanced Calculus", Prentice-Hall (1961), p.364.

Chapter 2

"A Critique of the Algebraic Quantization of Momenta"

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§1: Introduction.

We develop in this chapter a critique of the algebraic relationships which are commonly⁽¹⁻⁴⁾ regarded as obtaining between the quantum counterparts $Q(A)$ and $Q(B)$ of the classical observables A and B which stand in a known algebraic relationship one to the other; specifically we shall address the problem of whether and under what circumstances an algebra A of classical observables A defined over a Riemannian configuration manifold (M, G) generates a corresponding algebra $Q(A)$ whose elements are the quantum observables $Q(A)$ counterpart to the elements A of A , and are defined explicitly as self-adjoint operators over the natural Hilbert space of M , $\mathcal{L}^2_\rho(M)$.

To this end it is first necessary to generalise the concept of quantizability as defined for a momentum by statement [51] of chapter 1. We elect as our definition of quantizability of a general classical observable A the following axiom:

- [1] An observable A is quantizable if and only if it may be uniquely associated with an essentially self-adjoint operator $Q_0(A)$ defined on the domain of $C^\infty_0(M)$ functions.

The corresponding procedure of quantization of an observable A has therefore essentially two elements;

- [2] the identification of a symmetric differential operator $Q_0(A)$ generated by A and defined on the dense domain

$$DQ_0(A) = \{ \psi \in \mathcal{L}^2_\rho(M) \mid \psi \in C^\infty_0(M), Q_0(A)\psi \in \mathcal{L}^2_\rho(M) \} , \quad (1)$$

and

- [3] the determination of whether the operator $Q_0(A)$ is essentially self-adjoint, and, in the event that it is, the calculation of the explicit form of the corres-

ponding quantum observable $Q(A)$ from the formula

$$Q(A) = Q_0^\dagger(A) . \quad (2)$$

Thus, given the form of the observables $Q_0(A)$ generated by an algebra A of classical observables, we may by direct calculation explicitly construct the corresponding operators $Q(A)$, and hence determine whether a corresponding algebra $Q(A)$ of quantum observables $Q(A)$ exists and, in the event that it does, determine its structure.

By contrast the basis of the method of algebraic quantization is to postulate an isomorphism as obtaining between a given algebra A of classical observables and a corresponding algebra $Q(A)$ of quantum observables, and to employ the "rules of quantization" thus defined to determine the form, differential expression and domain of the operators of $\mathcal{L}_p^2(M)$ comprising the algebra $Q(A)$. Such a scheme, given symbolically by $A \leftrightarrow Q(A)$ induces a second algebra isomorphism between A and an algebra $Q_0(A)$ of symmetric operators whose elements $Q_0(A)$ are the restrictions to the domain $C_0^\infty(M)$ of the operators $Q(A)$, and whose operations coincide with the operations of $Q(A)$. We may therefore represent an algebraic quantization scheme by the sequence

$$A \leftrightarrow Q_0(A) \leftrightarrow Q(A) , \quad (3)$$

so that any proposed algebraic scheme of quantization must first define a consistent isomorphism $A \leftrightarrow Q_0(A)$.

Proceeding to discuss the problems which are encountered in any attempted realisation of such a quantization scheme we make two observations:

- [4] The existence of an isomorphism $A \leftrightarrow Q_0(A)$ serves (at least partially) to determine the operators $Q_0(A)$ so that an algebraic scheme of quantization may be used to identify a class of symmetric differential operators

to which the second stage, [3] of "geometric" quantization may be applied.

- [5] The process of geometric quantization can now be applied to generate the class of quantizable observables $B \subseteq A$ and the set $Q(B)$ of their quantum analogues. The scheme of geometric quantization will then be compatible with the generating algebraic scheme only if $Q(B)$ comprises an algebra isomorphic to A .

We thus perceive that a critique of the algebraic method of quantization can be obtained by comparison of the structure of the sets $Q(B)$ and $Q(A)$, that is by combining the algebraic structure of the symmetric operators $Q_0(A)$ with the axiom of quantizability [1] and the mode of quantization [2], [3] above. It is to the development for the observables linear in momenta of such a critique that we address ourselves in the remainder of this chapter.

§2: On the Algebraic Quantization of the Observables Linear in Momentum.

§2.1: On the algebraic quantization of the momenta.

We may introduce an algebra of momenta P on T^*M , the tangent bundle of a geodetically complete Riemannian manifold (M, G) , in accordance with the following theorem.

Theorem 1: On the Lie algebra of momenta.

Let P denote the set of momenta P whose associated vector fields are C^∞ , and define an algebra $(P, +, \cdot, \{, \})$ by the operations of addition, scalar multiplication, and by the Poisson bracket operation defined by the prescription¹

$$\{P(X), P(Y)\} = P([X, Y]) , \quad (4)$$

in which $P(X)$ is the momentum associated with the vector field X , and where $[X, Y]$ denotes the Lie or commutator bracket of the vector fields X and Y .

Then the algebra $P = (P, +, \cdot, \{, \})$ is an infinite-dimensional Lie algebra.

Proof: see appendix 1.

Let us enquire whether it is possible to introduce an algebraic scheme of quantization of the form $P \leftrightarrow Q_0(P) \leftrightarrow Q(P)$. To this end we first attempt the construction of a Lie algebra of "formal" quantum momenta $Q_0(P)$ isomorphic to P , a step realised concretely as follows:

Theorem 2: On the Lie algebra of formal quantum momenta.

Let P denote the Lie algebra of momenta, and let the map $Q_0: P \rightarrow Q_0(P)$ be defined by $P \mapsto Q_0(P)$, where $Q_0(P)$ is the symmetric differential operator on $\mathcal{L}_0^2(M)$ given by

$$Q_0(P) = -i\hbar(X + \frac{1}{2} \operatorname{div} X), \quad (5)$$

on the domain

$$DQ_0(P) = \{\psi \in \mathcal{L}_0^2(M) \mid \psi \in C_0^\infty(M), Q_0(P)\psi \in \mathcal{L}_0^2(M)\}. \quad (6)$$

Endow the set $Q_0(P)$ with the operations of operator addition and scalar multiplication, and with the (modified) bracket $\{, \}_0$ defined² by

¹ It is readily verified (Abraham and Marsden⁽⁵⁾) that this definition is equivalent to the usual coordinate based definition of the Poisson bracket

$$\{f, g\} = \frac{\partial f}{\partial x^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^i}$$

in which $P_1 = f = \xi_1^k p_k$, $P_2 = g = \xi_2^k p_k$.

² We shall quite generally define, for any operation A and B

$$\{A, B\}_0 = (-i\hbar)^{-1} [A, B],$$

as will be required in the sequel.

$$\{Q_0(P_1), Q_0(P_2)\}_0 = (-i\hbar)^{-1} [Q_0(P_1), Q_0(P_2)] , \quad (7)$$

in which $[,]$ denotes the commutator bracket of operators. Then $Q_0: P \rightarrow Q_0(P)$ is a Lie algebra isomorphism, and $Q_0(P) = (Q_0(P), +, \cdot, \{ , \}_0)$ is an infinite-dimensional Lie algebra isomorphic to P .

Proof: see appendix 1.

Turning now to the quantizability in accordance with axiom [1] of the formal quantum momenta $Q_0(P)$, we observe, by theorem 3 of chapter 1, that an operator $Q_0(P)$ is quantizable if and only if it is complete³, so that only the subset P_C of complete momenta is quantizable, and we are provided with the geometric quantization

$$P_C \leftrightarrow Q_0(P_C) \leftrightarrow Q(P_C) . \quad (8)$$

It is now clear that a Lie algebra isomorphism $Q: P \rightarrow Q(P)$ cannot, in general, be found; nor can a Lie algebra isomorphism between P_C and $Q(P_C)$, as is immediate from theorem 3, so that the algebraic scheme of quantization has no general applicability for the momenta.

Theorem 3: On the algebraic properties of P_C and $Q(P_C)$.

The subset P_C of the Lie algebra P of momenta is not a Lie subalgebra of P ; specifically the set P_C is closed neither under addition, nor under the action of the Poisson bracket. Hence, since the quantization map Q is bijective, it is immediate that the set $Q(P_C)$ cannot constitute a Lie algebra.

Proof: see appendix 1.

³ Here strictly we must have complete except on a set of measure zero, so that we may interpret "complete" in this broader sense.

This result clearly places severe restrictions upon the utility of any algebraic scheme of quantization for the momenta; for the non-closure of P_C under the basic operations of classical mechanics, addition and Lie (Poisson) derivation, renders an algebra preserving isomorphism $P_C \leftrightarrow Q(P_C)$ incompatible with the geometrical quantization procedure of Mackey. We may, nevertheless, discover some useful "laws of quantization" which obtain when the result of an algebraic operation on the elements of P_C is itself within P_C , among which are the following:

Theorem 4: The basic laws of quantization of the complete momenta.

For all elements $P_1, P_2 \in P_C$ we have the following propositions:

$$P_1 + P_2 \in P_C \Rightarrow Q(P_1 + P_2) = (Q(P_1) + Q(P_2))^{\dagger}; \quad (9)$$

$$\{P_1, P_2\} \in P_C \Rightarrow Q(\{P_1, P_2\}) = \{Q(P_1), Q(P_2)\}_0^{\dagger}. \quad (10)$$

Proof: see appendix 1.

Thus we may introduce the operations of addition and Lie derivation on $Q(P_C)$ related to those already defined by the prescriptions

$$Q(P_1 + P_2) = Q(P_1) \boxplus Q(P_2) = (Q(P_1) + Q(P_2))^{\dagger}, \quad (11)$$

$$Q(\{P_1, P_2\}) = \{Q(P_1), Q(P_2)\} = \{Q(P_1), Q(P_2)\}_0^{\dagger}. \quad (12)$$

These operators then define, for a suitable class of the complete momenta P_C , an algebraic structure on the corresponding quantum observables $Q(P_C)$, so that it is natural to enquire whether and under what conditions there exist Lie subalgebras of P contained within P_C ; for such subalgebras have corresponding isomorphic quantum Lie algebras induced by the quantization operation. There are in fact several identifiable such subalgebras all of which we shall collect into theorem.

Theorem 5: Some particular Lie subalgebras of P within P_C .

The following sets of complete momenta define Lie subalgebras of the Lie algebra P of momenta of a geodetically complete Riemannian manifold (M, G) .

[6] Any set of mutually commuting complete momenta, symbolically

$$\{P_\mu \in P_C | \{P_\mu, P_\nu\} = 0 \quad \forall \mu, \nu\} . \quad (13)$$

[7] The set of all Killing momenta P_K defined by

$$P_K = \{P \in P | P = P(X), D_X G = 0\} . \quad (14)$$

[8] The set of all "compact" momenta P_K defined as

$$P_K = \{P \in P | P = P(X), \text{supp } X \text{ is compact in } M\} . \quad (15)$$

Proof: see appendix 1.

Moreover, for the special case of a compact manifold (M, G) we have the result:

Theorem 6: On the momenta of a compact manifold.

Every $P \in P$ defined over a compact manifold (M, G) is complete.

Proof: Brickell and Clarke⁽⁶⁾.

Whence it follows that $P = P_C$ is, in this case, a Lie algebra of quantizable momenta isomorphic to the induced quantum algebra $Q(P)$ and the algebraic quantization scheme is fully realisable.

Let us parenthetically remark that, as is demonstrated by Wan and Viazminsky^(7,8), the algebraic properties of the Killing momenta on a space of constant curvature are sufficient to determine by means of the

following device the free quantum Hamiltonian. Let P_μ , $\mu \in [1, \frac{1}{2}n(n+1)]$ denote a maximal set of linearly independent Killing momenta on a space M of constant curvature and of dimension n , and define the structure constants of the associated Lie algebra P_K by the equations

$$\{P_\mu, P_\nu\} = c_{\mu\nu}^k P_K, \quad (16)$$

and the metric tensor $G_{\mu\nu}$ of the algebra by the prescription

$$G_{\mu\nu} = c_{\mu\lambda}^k c_{\nu k}^\lambda. \quad (17)$$

Then if we require that $Q(H)$, the free quantum Hamiltonian, is a second order differential operator satisfying the commutation relations

$$\{Q(H), Q(P_\mu)\} = 0, \quad (18)$$

it follows that

$$Q(H) = \alpha G^{\mu\nu} Q(P_\mu) Q(P_\nu) + \beta = -\alpha \hbar^2 \nabla^2 + \beta, \quad (19)$$

where α and β are real constants, a result which differs but trivially from the Laplacian operator. This example illustrates well the utility and strength of an algebraic approach in appropriate special cases where a high degree of "symmetry" is present in the underlying physical system.

The results and theorems of this section comprise a clear statement of the incompatibility which obtains between the geometrical scheme of quantization based upon essential self-adjointness as the criterion of quantizability, and an algebraic scheme based upon the isomorphism of the classical and quantum algebras. In the case of the momenta moreover the ascendancy of the geometrical procedure is, especially in view of chapter 1, well attested, so that, other than in certain particularly convenient spaces, such as those which are compact or of constant curvature, the algebraic structure of the momenta is of comparatively little constructional value.

§2.2: The geometric quantization of observables linear in momentum.

We address in this section the problem of the quantization, in accordance with axiom 1, of the observables linear in momentum, which we denote symbolically by $P+f$, and define as follows:

[9] An observable linear in momentum (linear momentum observable) is a map $P+f:T^*M \rightarrow \mathcal{R}$ given by the prescription,

$$\forall x \in T^*M \quad (P+f)(x) = P(x) + f(\pi(x)) , \quad (20)$$

in which P is a C^∞ momentum, f is a C^∞ function on M , and $\pi:T^*M \rightarrow M$ is the natural projection defined by the coordinate representation $\pi(x^i, p_i) = (x^i)$.

It is immediately clear that in a coordinate chart $\{(x^i, p_i) | i \in [1, n]\}$ of T^*M the map $P+f$ has, in accordance with the intuitive force of the term "observable linear in momentum", the form $\xi^i(x^j)p_i + f(x^j)$. We shall assume that the formal quantization of $P+f$ is in accordance with the rule of quantization

$$Q_o(P+f) = Q_o(P) + Q_o(f) , \quad (21)$$

or equivalently that the operator $Q_o(P+f)$ has the explicit form

$$Q_o(P+f) = -i\hbar(X + \frac{1}{2} \operatorname{div} X + i\hbar^{-1} f) , \quad (22)$$

on the domain

$$DQ_o(P+f) = \{\psi \in \mathcal{L}^2_\rho(M) | \psi \in C^\infty_o(M), Q_o(P+f)\psi \in \mathcal{L}^2_\rho(M)\} . \quad (23)$$

The conditions under which the forms $P+f$ are quantizable, and the explicit representation of the corresponding self-adjoint quantum analogues $Q(P+f)$, comprise the following key theorem.

Theorem 7: On the quantization of observables linear in momentum.

Let $P+f$ denote an observable linear in momentum defined over a Riemannian manifold (M,G) , and let X denote the C^∞ vector field on M associated with the momentum P ; then

[10] $P+f$ is quantizable if and only if P is quantizable, and

[11] $Q(P+f)$ has the explicit representation

$$Q(P+f) = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X + i\hbar^{-1} f) , \quad (24)$$

on the domain

$$DQ(P+f) = \{ \psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C^1(X,M), Q(P+f)\psi \in \mathcal{L}_\rho^2(M) \} , \quad (25)$$

and hence obeys the rule of correspondence

$$Q(P+f) = Q(P) + Q(f) . \quad (26)$$

Proof: see appendix 2.

In addition it has proved possible to determine the precise form of the unitary transformations U_t generated by an observable $Q(P+f)$ in accordance with the equation

$$U_t = \exp(-i/\hbar Q(P+f)t) ; \quad (27)$$

specifically we have the following theorem.

Theorem 8: On the unitary transformations U_t induced by a linear momentum observable.

Let $P+f$ be an observable linear in momentum generated by a complete momentum P , and let Φ_t^* denote the pull-back of the flow mapping Φ_t of the corresponding vector

field X .

Define the operators $U_t: \mathcal{L}^2_\rho(M) \rightarrow \mathcal{L}^2_\rho(M)$, $t \in \mathbb{R}$ by

$$U_t = \exp(i\omega(f,t)/\hbar) (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^* \psi, \quad (28)$$

in which Φ_t^* denotes the pull-back of Φ_t acting on the Riemannian density ρ or a state ψ as appropriate, and in which $\omega(f,t) \in C^1(X,M)$ is a function on M defined formally by the system

$$\omega(f,t) = (\Phi_t^* - 1)g(f), \quad D_X g = f, \quad (29)$$

and precisely as in appendix 2.

Then the set $\{U_t | t \in \mathbb{R}\}$ comprises a one-parameter group of unitary transformations on M .

Proof: See appendix 1 of chapter 1 for a definition of $\Phi_t^* \rho / \rho$, and appendix 2 for the proof.

Note in particular that when $f = 0$, $\omega(f,t) = 0$, so that the unitary transformations generated by $Q(P+f)$ are related to those generated by $Q(P)$ by the formula

$$U_t^{Q(P+f)} = \exp(i\omega(f,t)/\hbar) U_t^{Q(P)}. \quad (30)$$

In the special case⁴ where the solution $g(f): D_X g = f$ defines a function $g \in C^1(X,M)$, then we have the following result.

⁴ It should be particularly noted that, contrary to first expectation, not every function $f \in C^\infty(M)$ defines a function $g \in C^1(X,M)$ such that $D_X g = f$, as can be seen by considering an example, say, $X = y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y}$, $f = 1$, on \mathbb{R}^2 with the usual metric.

Theorem 9: The case of unitary equivalence of $Q(P)$ and $Q(P+f)$.

Whenever the function $g(f)$ defined by $D_X g = f$ is of class $C^1(X, M)$, then the unitary operators $U_t^{Q(P+f)}$ are related to the corresponding operators $U_t^{Q(P)}$ by the unitary transformation

$$U_t^{Q(P+f)} = e^{-ig/\hbar} U_t^{Q(P)} e^{+ig/\hbar}. \quad (31)$$

Moreover we have by differentiation or by explicit calculation that

$$Q(P+f) = e^{-ig/\hbar} Q(P) e^{+ig/\hbar}, \quad (32)$$

so that $Q(P+f)$ being unitarily equivalent to $Q(P)$ has the same spectrum, the spectral functions being related by the equality

$$E_{(\lambda)}^{Q(P+f)} = e^{-ig/\hbar} E_{(\lambda)}^{Q(P)} e^{+ig/\hbar}. \quad (33)$$

Proof: see appendix 2.

The results outlined in theorem 9 which relate $Q(P)$ to $Q(P+f)$ by a unitary transformation must be regarded as exceptional, however; for in general the spectrum and spectral operator of $Q(P+f)$ differ radically from those of $Q(P)$. We may illustrate these remarks by recourse to the favoured example of the angular momentum observable L_z on \mathbb{R}^2 with the usual metric. The spectrum of $Q(L_z)$ is wholly discrete of eigenfunctions

$$\psi_n(r, \theta) = \alpha_n(r) \exp(ip_n \theta/\hbar), \quad n \in \mathbb{Z} \quad (34)$$

where (r, θ) denotes the plane polar coordinates of a point of \mathbb{R}^2 , and where $\alpha_n(r)$ is any function such that ψ_n is normalisable, and of eigenvalues

$$p_n = n\hbar, \quad n \in \mathbb{Z}. \quad (35)$$

Consider now the eigenfunctions of the quantum observable $Q(L_z + f)$, $f \in C^\infty(\mathbb{R}^2)$. We have the following formal "eigenfunctions"

$$\psi_\mu(r, \theta) = \alpha_\mu(r) e^{i\mu/\hbar\theta} \exp(i/\hbar \int_0^\theta f(r, \theta) d\theta) . \quad (36)$$

True eigenfunctions corresponding to points of the discrete spectrum exist if and only if the " θ -mean" of $f(r, \theta)$,

$$\langle f \rangle = 1/2\pi \int_0^{2\pi} f(r, \theta) d\theta , \quad (37)$$

is an absolute constant, when the spectrum of eigenvalues is given by

$$\mu_n = n\hbar - \langle f \rangle , \quad n \in \mathbb{Z}, \quad (38)$$

and corresponds to the spectrum of $Q(L_z)$ "phase-shifted" by $-\langle f \rangle$.

Otherwise there are no eigenfunctions of $Q(L_z + f)$ and the spectrum is wholly continuous. Hence it is immediate that in general, else when $\langle f \rangle = 0$, the spectrum of $Q(L_z + f)$ is not that of $Q(L_z)$, or even, except when $\langle f \rangle$ is constant, simply related thereto, and hence that the observables $Q(L_z + f)$ are non-trivially distinct from $Q(L_z)$. As a final remark we note that when the vector field X induced by $Q(P + f)$ has no closed maximal integral curves then $g(f) \in C^1(X, M)$ and hence the results of theorem 9 obtain.

When viewed alternatively theorem 9 is seen to contain a statement of when a change of quantum mechanical "representation"⁵ can be effected such as will transform the observable $Q(P + f)$ linear in momentum into a "pure" momentum $Q(\bar{P})$, such a transformation being induced by the unitary operator $U_f = e^{ig/\hbar}$ when and only when g is of class $C^1(X, M)$. Correspondingly we may enquire whether and under what conditions such a transformation of "representation" can be carried out within classical mechanics. Here the kernel observation is that, formally at least, the observable linear in momentum $P + f$ of coordinate representation

⁵ The term "representation" is here used as in Messiah⁽⁹⁾.

$\xi^i(q^j)p_i$ can be transformed to a "pure" momentum $\bar{P} = \xi^i(\bar{q}^j)\bar{p}_i$ by the action of the canonical transformation⁽¹⁰⁾ prescribed in terms of the generating function⁽¹¹⁾

$$F(q^i, \bar{q}^j, p_i, \bar{p}_j) = q^i \bar{p}_i - g(q^i), \quad (39)$$

by the differential equations

$$p_i = \frac{\partial F}{\partial q^i}, \quad \bar{q}^i = \frac{\partial F}{\partial \bar{p}_i}. \quad (40)$$

We collect the results of our analysis in the following theorem.

Theorem 10: On the transformation of observables linear in momentum into "pure" momenta.

A transformation taking the usual Schrödinger "representation" of a quantum system, to a unitarily equivalent "representation", and satisfying the condition that, for a particular observable linear in momentum, $Q(P+f)$ is transformed into a "pure" momentum $Q(\bar{P})$, exists if and only if a function $g(f)$ exists such that $g \in C^1(X, M)$ and $D_X g = f$. When it exists such a transformation of representation is determined by the unitary operator $U_f = e^{ig/\hbar}$, the state vector ψ transforming as

$$\psi \rightarrow U_f \psi, \quad (41)$$

and the operators Ω transforming as

$$\Omega \rightarrow U_f \Omega U_f^{-1}. \quad (42)$$

Moreover if $g \in C^1(M)$, then there exists a corresponding transformation of the classical representation of the system induced by the generating function F of (39) above,

such that the observable $P + f$ linear in momentum is transferred to the "pure" momentum \bar{P} as follows:

$$P + f = \xi^i(q^j) p_i + f(q^j) = \xi^i(\bar{q}^j) \bar{p}_i = \bar{P} . \quad (43)$$

Proof: corollary to theorem 9 and the equations (39) and (40).

§2.3: On the algebraic quantization of observables linear in momentum.

We address in this section the algebraic properties which obtain between the observables linear in momentum and between their corresponding quantum analogues, and begin by defining the product ϕP of a momentum P and a function ϕ on M , and the Poisson bracket appropriate to observables of the form $P + f$.

[12] The product ϕP_X of the momentum P_X with a function ϕ on M is the momentum prescribed by

$$\phi P_X = P_{\phi X} , \quad (44)$$

where generally P_X denotes the momentum associated with the vector field X .

[13] The Poisson bracket of two observables linear in momentum is given by

$$\{P_1 + f_1, P_2 + f_2\} = \{P_1, P_2\} + X_1 f_2 - X_2 f_1 , \quad (45)$$

where X_i is the vector field associated with the momentum P_i and where $\{P_1, P_2\}$ is as defined in (4).

These operations, together with the obvious addition and scalar multiplication enable the construction of an algebra on the set

$$P + F = \{ \phi P + f | P \in P; \phi, f \in C^\infty(M) \} , \quad (46)$$

of the following structure:

Theorem 11: On the Lie algebra of observables linear in momentum.

The set $P+F$ when endowed with the operations of addition and scalar multiplication, and the Lie derivative generated by the Poisson bracket (45) is an infinite-dimensional Lie algebra.

Proof: see appendix 3.

Similarly the operator of formal quantization Q_o defined by the algebraic relation

$$Q_o(P+f) = Q_o(P) + Q_o(f) , \quad (47)$$

induces an algebraic structure on the corresponding symmetric operators $Q_o(\phi P+f)$ as follows.

Theorem 12: On the Lie algebra of formal quantum observables linear in momentum.

The set $Q_o(P+F)$ endowed with operator addition, scalar multiplication, and the (modified) commutator bracket

$$\{Q_o(P_1+f_1), Q_o(P_2+f_2)\}_o = (-i\hbar)^{-1} [Q_o(P_1)+f_1, Q_o(P_2)+f_2] , \quad (48)$$

in which $[,]$ denotes the commutator bracket of operators, defines an infinite-dimensional Lie algebra isomorphic to $P+F$. Additionally the map Q_o has the property

$$Q_o(\phi P) = \frac{1}{2} [Q_o(\phi), Q_o(P)]_+^o , \quad (49)$$

where $[,]_+^o$ denotes the anticommutator bracket.

Proof: see appendix 3.

Turning now to the construction of an algebraic structure on the set of quantum observables $Q(P_C^{+F})$ generated from the quantization operator Q , in accordance with axiom [1] and result [10], by the set P_C^{+F} , we immediately perceive that, as with the momenta, the set P_C^{+F} is closed neither under addition nor under the Poisson bracket, and that therefore the algebraic method of quantization has for the observables linear in momentum no general applicability. However in those cases where the result of an algebraic operation on the elements of P_C^{+F} is itself an element of P_C^{+F} , the following relationships hold:

Theorem 13: The basic laws of quantization for observables linear in momentum.

For all elements P_1, P_2 of P_C , and all C^∞ functions ϕ, f_1, f_2 of M , we have the following propositions:

$$P_1 + P_2 \in P_C \Rightarrow Q(P_1 + f_1 + P_2 + f_2) = (Q(P_1 + f_1) + Q(P_2 + f_2))^{\dagger}; \quad (50)$$

$$\{P_1, P_2\} \in P_C \Rightarrow Q\{P_1 + f_1, P_2 + f_2\} = \{Q(P_1), Q(P_2)\}_0^{\dagger} + X_1 f_2 - X_2 f_1; \quad (51)$$

$$\phi P \in P_C \Rightarrow Q(\phi P) = (\frac{1}{2}[Q(\phi), Q(P)]_+^0)^{\dagger}; \quad (52)$$

in which as above $P_i = P(X_i)$.

Proof: see appendix 3.

We may now introduce operations of addition, Lie derivation, and anti-commutation on $Q(P_C^{+F})$ defined by the prescriptions;

$$Q(P_1 + f_1) \boxplus Q(P_2 + f_2) = (Q(P_1) + Q(P_2)) , \quad (53)$$

$$\{Q(P_1 + f_1), Q(P_2 + f_2)\} = \{Q(P_1 + f_1), Q(P_2 + f_2)\}_0^{\dagger}, \quad (54)$$

$$[Q(\phi), Q(P)]_+ = ([Q(\phi), Q(P)]_+^0)^{\dagger}. \quad (55)$$

These operators then define for a suitable subclass of the observables

of $P_C + F$ an algebraic structure on the corresponding set of quantum analogues, so that, given a Lie subalgebra of $P + F$ contained within $P_C + F$, an isomorphic Lie algebra of quantum operators is generated by the operation of quantization Q and the definitions (53) - (55).

Finally we present in the context of a theorem some examples of such Lie subalgebras.

Theorem 14: Some particular Lie subalgebras of $P_C + F$.

The following sets define Lie subalgebras of the Lie algebra $P + F$ of observables linear in momentum of a geodetically complete Riemannian manifold (M, G) .

[14] Any set of mutually commuting linear momentum observables,

$$\{P_\mu + f | \{P_\mu, P_\nu\} = 0, \{P_\mu, f\} = 0\} . \quad (56)$$

[15] The set $P_K + F$ of observables generated by the Killing momenta,

$$P_K + F = \{P + f | P \in P_K, f \in C^\infty(M)\} . \quad (57)$$

[16] The set of all "compact" observables linear in momentum,

$$P_K + F = \{P + f | P \in P_K, f \in C^\infty(M)\} . \quad (58)$$

Finally for the case of a compact manifold we have that

[17] the set $P + F = P_C + F$ is a quantizable Lie algebra of observables.

Proof: see appendix 3.

§3: Conclusion and Prospect.

The analyses of this chapter have in some detail elucidated under what conditions hold, and of what type are, the algebraic relationships between the quantum observables linear in momentum⁶.

The principal conclusions are the following;

[18] that an algebra of quantum momenta isomorphic to a classical Lie algebra P of momenta can be constructed if and only if the set P is contained in the set, P_C , of complete momenta, itself determined as the class of geometrically quantizable momenta,

[19] that an observable, $P+f$, linear in momentum is geometrically quantizable if and only if its component momentum P is complete, and finally

[20] that an algebra $P+F$ of observables linear in momentum generates an isomorphic quantum algebra if and only if the set P of component momenta is a subset of P_C .

Thus we perceive that neither an algebraic approach to the problem of the quantization of, nor any general algebraic manipulation of the momenta can be undertaken in a general Riemannian space (M,G) .

Turning now to the prospect of future development based upon the content of this chapter, we note that, whereas any further comparative study of the algebraic and geometrical methods of quantization needs await the development of a geometrical quantization procedure encompassing a larger class of observables, there nevertheless remains at least one area of research which is accessible in the medium term future. This area of research consists of

⁶ It may be of interest to note that some results concerning the algebraic approach when applied to the "entire" class of classical observables may be found in Abraham and Marsden⁽¹²⁾ and also in Van Hove⁽¹³⁾.

- [21] the construction of a theory of measurement of the observables linear in momentum, in both the classical and quantum cases, so as to develop concepts of classical and quantum global measurability analogous to those of chapter 1, and
- [22] the comparison for an observable linear in momentum of the conditions for global measurability with those already derived for geometrical quantizability, so as to determine whether a physically based axiom of quantizability, similar to [51] of chapter 1, may be introduced.

In conclusion we may say that the geometrical criterion of essential self-adjointness has resulted in the partitioning of the observables linear in momentum into two distinct subclasses. It is to be regretted that the class P_C^{+F} of quantizable momenta is not, in general, closed under addition or the action of the Poisson bracket.

References to Chapter 2

References to Chapter 2

- 1: Bloore F.J.: "Quantization on a Riemannian Manifold" Colloques Internationaux C.N.R.S. No.237 - Geometrie symplectique et physique mathematique, 300-303.
- 2: Bloore F.J. and Routh L.: "The Covariant Form for Quantum-Mechanical Operators which are Quadratic in Momentum", Nuovo Cimento 25B (1975) 78-84.
- 3: Segal I.E.: "Quantization of Nonlinear Systems", J. Math. Phys. 1 (1960) 468-488.
- 4: Castellani L.: "Quantization Rules and Dirac's Correspondence", Nuovo Cimento 48A (1978) 359-368.
- 5: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), §5.4, p.429.
- 6: Brickell F. and Clark R.S.: "Differentiable Manifolds", Van Nostrand Reinhold (1970), proposition 8.2.6, p.139.
- 7: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977) 1030-.
- 8: Wan K.K. and Viazminsky C.: "Lie Algebra and the quantization of momenta and the Hamiltonian", J. Phys. A 12 (1979), 643-647.
- 9: Messiah A.: "Quantum Mechanics", volume 1, North Holland Publishing Company (1961), Chapt.8, §9, §10, pp311-317.
- 10: Goldstein H.: "Classical Mechanics", Addison Wesley (1972), Chapt.8 esp. pp240-241.
- 11: Sudarshan E.C.G. and Mukunda N.: "Classical Dynamics: A Modern Perspective", Wiley and Sons (1974), pp57-58.
- 12: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), §5.4, pp434-441.
- 13: Van Hove L.: "Sur certaines représentations unitaires d'un groupe infini de transformations", Mem. de l'Acad. Roy. de Belgique (Classe des Sci.) 26, 61-102.

Appendices to Chapter 2

Appendix 1: On the Algebraic Quantization of Observables Linear in Momentum.

[1] Theorem 1: On the Lie algebra of momenta.

Proof: The map P acting on the C^∞ vector fields X and defined by $P(X) = W_0(X)$, where $W_0 = p_i dx^i$ is the fundamental linear form^(a1) of M , constitutes a linear isomorphism between the C^∞ vector fields X and the corresponding momenta $P(X)$ of M satisfying

$$P([X,Y]) = \{P(X), P(Y)\} ; \quad (A1.1)$$

that is P is a Lie algebra isomorphism. Hence it suffices to observe^(a2) that the set of C^∞ vector fields on M , when endowed with the usual addition, scalar multiplication, and the Lie bracket $[,]$, comprise an infinite-dimensional Lie algebra.

[2] Theorem 2: On the Lie algebra of formal quantum momenta.

Proof: As above observe that the map $Q_0: P \rightarrow Q_0(P)$ defined by the action of the formal quantization operator is an isomorphic linear map satisfying

$$Q_0(\{P_1, P_2\}) = \{Q_0(P_1), Q_0(P_2)\}_0 , \quad (A1.2)$$

and that P is, by theorem 1, an infinite-dimensional Lie algebra, so that Q_0 is a Lie algebra isomorphism, and $Q_0(P)$ is itself an infinite-dimensional Lie algebra isomorphic to P .

[3] Theorem 3: On the algebraic properties of P_C and $Q(P_C)$.

Proof: We simply demonstrate by counter-example on $(\mathbb{R}^2, 1)$ that in general neither the sum nor the commutator bracket of two C^∞ complete vector fields X and Y is complete.

example 1: $X = y^2 \partial / \partial x$, $Y = x^2 \partial / \partial y$.

These vector fields are clearly C^∞ and complete having the flows

$$\Phi_t^X(x, y) = (x + y^2 t, y), \quad \Phi_t^Y(x, y) = (x, y + x^2 t), \quad t \in \mathbb{R}. \quad (\text{A1.3})$$

Their commutator bracket has the explicit form

$$[X, Y] = 2xy \left(y \frac{\partial}{\partial y} - x \frac{\partial}{\partial x} \right), \quad (\text{A1.4})$$

and hence the corresponding flow $\Phi_t^{[X, Y]}$ is determined by the differential equations

$$dx/dt = -2x^2 y, \quad dy/dt = 2xy^2, \quad (\text{A1.5})$$

which have the general solutions

$$x^2 = x_0^2 / (1 + tx_0 y_0), \quad y^2 = y_0^2 / (1 + tx_0 y_0), \quad (\text{A1.6})$$

where (x_0, y_0) is the initial point at $t = 0$. It is now immediate that real-valued solutions exist only when $(1 + tx_0 y_0) \geq 0$ and thus that $[X, Y]$ is incomplete.

example 2: $X = y \partial / \partial x$, $Y = -e^{-2x} \partial / \partial y$.

These vector fields are clearly complete and have corresponding flows

$$\Phi_t^X(x, y) = (x + yt, y), \quad \Phi_t^Y(x, y) = (x, y - e^{-2x} t). \quad (\text{A1.7})$$

The sum

$$X + Y = y \partial / \partial x - e^{-2x} \partial / \partial y, \quad (\text{A1.8})$$

generates the corresponding flow ϕ_t^{X+Y} via the differential equations

$$\frac{dx}{dt} = y, \quad \frac{dy}{dt} = -e^{-2x}. \quad (\text{A1.9})$$

Integration then yields the following solutions,

$$x = \ln(y^2 - \omega^2), \quad \omega^2 = y_0^2 - e^{-2x_0}, \quad (\text{A1.10})$$

$$y(t) = \omega \left[\frac{(\omega + y_0)e^{2\omega t} - (\omega - y_0)}{(\omega + y_0)e^{2\omega t} + (\omega - y_0)} \right],$$

so that $\omega \in \mathbb{C}$ in general. It is now readily perceived that when $(\omega + y_0)e^{2\omega t} + (\omega - y_0) = 0$, then t assumes a finite value, the precise value being determined by whether ω is real or imaginary. Thus the vector field $X+Y$ is manifestly incomplete.

[4] Theorem 4: The basic "laws of quantization" of the complete momenta.

Proof: $Q_0(P_1)$, $Q_0(P_2)$, $Q_0(P_1+P_2)$, $Q_0(\{P_1, P_2\})$ are by hypothesis essentially self-adjoint, so that we have the following inequalities:

$$\begin{aligned} (Q(P_1) + Q(P_2))^{\dagger\dagger} &\supseteq (Q_0(P_1) + Q_0(P_2))^{\dagger\dagger} = Q_0^{\dagger\dagger}(P_1+P_2) = \\ &Q_0^{\dagger}(P_1+P_2) \supseteq (Q(P_1) + Q(P_2))^{\dagger}; \end{aligned} \quad (\text{A1.11})$$

$$\begin{aligned} \{Q(P_1), Q(P_2)\}_0^{\dagger\dagger} &\supseteq \{Q_0(P_1), Q_0(P_2)\}_0^{\dagger\dagger} = Q_0^{\dagger\dagger}(\{P_1, P_2\}) = \\ &Q_0^{\dagger}(\{P_1, P_2\}) \supseteq \{Q(P_1), Q(P_2)\}_0^{\dagger}. \end{aligned} \quad (\text{A1.12})$$

Hence, since for all symmetric operators Ω , $\Omega^{\dagger\dagger} \subseteq \Omega^{\dagger}$, we deduce that $Q(P_1) + Q(P_2)$ and $\{Q(P_1), Q(P_2)\}$ are essentially self-adjoint and that therefore their adjoints are well-formed self-adjoint operators respectively equal to $Q(P_1+P_2)$ and $Q\{P_1, P_2\}$ as required.

[5] Theorem 5: Some particular Lie sub-algebras of P .

Proof: part 1: Any set of mutually commuting complete momenta

$$\{P_\mu \in P_C | \{P_\mu, P_\nu\} = 0, \quad \forall \mu, \nu\}, \quad (A1.13)$$

form a Lie algebra.

Proof: Let $\Phi_t^P: M \rightarrow M$ be the flow associated with the momentum P_μ ; then

$$\Phi_t^{\alpha P_\mu} = \Phi_{\alpha t}^{P_\mu}, \quad \Phi_t^{P_\mu + P_\nu} = \Phi_t^{P_\mu} \circ \Phi_t^{P_\nu}, \quad (A1.14)$$

the latter being demonstrated in Abraham and Marsden^(a3), so that the set (A1.13) is closed under addition and scalar multiplication, its closure under the Poisson bracket being trivial. Hence we have demonstrated that the set above defines a Lie sub-algebra of P .

part 2: The set P_K of all Killing momenta on a geodetically complete Riemannian manifold (M, G) forms a Lie algebra.

Proof: Since the Killing vectors associated with the Killing momenta are closed under the Lie bracket, and scalar multiplication, it suffices to show that all Killing vectors on a geodetically complete manifold (M, G) are complete. Let Φ_t denote the flow-map associated with a Killing vector field X on M , and let x_0 be a point of M . Then there are four possible distinct categorisations of x_0 :

(i) x_0 is a critical point of X when

$$\Phi_t(x_0) = x_0 \quad \forall t \in \mathbb{R}.$$

(ii) x_0 lies on a closed integral curve

$$\Omega(x_0) \text{ of } X \text{ when } \Phi_t(x_0) = \Phi_{t+\tau}(x_0), \\ \tau \in \mathbb{R}^+, \quad \forall t \in \mathbb{R}.$$

(iii) x_0 lies on an integral curve $\Omega(x_0)$

which "begins" and "ends" on critical points, when the C^∞ character of the field assures that $\Phi_t(x_0) \in M \quad \forall t \in \mathbb{R}$.

(iv) x_0 lies on an open (semi-open) integral curve.

Of these cases only the last need be considered further. We have that for a Killing vector field the arc-length parametrisation of the (semi-) infinite integral curve $\Omega(x_0)$ is related to the t -parametrisation by

$$s = \int_0^t b_1^1(t) dt = s_0(\Omega(x_0))t, \quad (\text{A1.15})$$

where s_0 is a constant on each integral curve $\Omega(x_0)$ as is demonstrated in appendix 10 of chapter 1. Hence, denoting by $d(x,y)$ the metrical (least) distance between two points x and y of M , we have that for all values of t in its range along $\Omega(x_0)$,

$$d(\Phi_t(x_0), x_0) \leq s(\Omega(x_0), \Phi_t(x_0), x_0) = s_0 t, \quad (\text{A1.16})$$

so that points at any finite " t -distance" from x_0 are finitely remote in real distance. But

$\Omega(x_0)$ has no critical point for $t > 0$, say,
 and thus has no end-point $\Phi_\infty(x_0) \in M$, so that,
 $\Omega(x_0)$ cannot end within M and hence must
 terminate as $\Phi_t(x_0)$ "approaches infinity".
 This last implies by (A1.16) that $t \rightarrow \infty$ so
 that $\Omega(x_0)$ is positively complete. A similar
 argument will apply for $t < 0$ so that $\Omega(x_0)$ is
 complete as required.

part 3: The set P_K of all "compact" momenta form a Lie algebra.

Proof: see Abraham and Marsden^(a4).

Appendix 2: The Quantization of Observables Linear in Momentum.

We give in this appendix a systematic treatment of the quantization of the observables linear in momentum in the course of which we shall demonstrate the theorems 7, 8, and 9 of chapter 2. We shall adopt as far as possible the symbolism of appendix 1 of chapter 1 so as to facilitate comparison, and begin our discussion with two technical lemmata.

Lemma 2.1: Let X be a C^∞ vector field on the Riemannian manifold (M, G) ; let $\Phi_t^*: \mathcal{L}_\rho^2(M) \rightarrow \mathcal{L}_\rho^2(M)$ denote the pull-back of functions under the flow Φ_t of X , and denote by $D_X\psi$ the Lie derivative of ψ with respect to X . Then

$$[D_X, \Phi_t^*] = 0, \quad (\text{A2.1})$$

and moreover if $\psi \in C^1(X, M)$ then $\Phi_t^*\psi \in C^1(X, M)$.

Proof: We have $\forall \psi \in \mathcal{L}_\rho^2(M): \Phi_t^*\psi \in C^1(X, M)$ that the following equalities hold

$$D_X(\Phi_t^*\psi) = \lim_{s \rightarrow 0} s^{-1} [\Phi_s^* \circ \Phi_t^*\psi - \Phi_t^*\psi] = \lim_{s \rightarrow 0} \Phi_t^*(\Phi_s^*\psi - \psi)s^{-1}; \quad (\text{A2.2})$$

thus, provided that $\psi \in C^1(X, M)$, we have by continuity of Φ_t^* that

$$D_X(\Phi_t^*\psi) = \Phi_t^*(\lim_{s \rightarrow 0} s^{-1} [\Phi_s^*\psi - \psi]) = \Phi_t^*D_X\psi, \quad (\text{A2.3})$$

and hence immediately $[D_X, \Phi_t^*] = 0$. Finally we observe that if $\psi \in C^1(X, M)$ then $D_X\psi$ exists, and hence, by continuity of $\Phi_t^*, D_X(\Phi_t^*\psi)$ exists, so that $\Phi_t^*\psi \in C^1(X, M)$.

Lemma 2.2: On the definition and properties of the function $\omega(f, t)$.
 Let X be a C^∞ complete vector field on M ; let f be a C^∞ function on M ,
 and let Φ_t^* denote the pull-back of functions under the flow Φ_t of X .
 Then the quantity $\omega(f, r): M \rightarrow M$ defined by the integral

$$\omega(f, r)(x) = \int_0^r (\Phi_t^* f)(x) dt, \quad \forall x \in M \quad (A2.4)$$

in which r is a real-valued parameter, is a $C^\infty(X, M)$ function on M .
 Moreover $\omega(f, r)$ has the following properties:

[1] $\omega(f, r)$ is r -differentiable and

$$d\omega(f, r)/dr = \Phi_r^* f; \quad (A2.5)$$

$$[2] \quad D_X^n \omega(f, r) = (\Phi_r^* - 1) D_X^{n-1} f, \quad n \in N; \quad (A2.6)$$

$$[3] \quad \Phi_s^* \omega(f, r) = \omega(f, r+s) - \omega(f, s). \quad (A2.7)$$

Proof: We proceed immediately to demonstrate the differentiability of $\omega(f, r)$, and first show that $\omega(f, r) \in C^1(X, M)$. Consider the Lie derivative $D_X \omega(f, r)$ evaluated at some x ; we have by definition that

$$\begin{aligned} D_X \omega(f, r) &= \lim_{u \rightarrow 0} u^{-1} [\Phi_u^* \int_0^r (\Phi_s^* f)(x) ds - \int_0^r (\Phi_s^* f)(x) ds] \quad (A2.8) \\ &= \lim_{u \rightarrow 0} u^{-1} [\int_0^r (\Phi_{u+s}^* f)(x) ds - \int_0^r (\Phi_s^* f)(x) ds], \end{aligned}$$

and hence by change of variable that

$$\begin{aligned} D_X \omega(f, r) &= \lim_{u \rightarrow 0} u^{-1} [\int_u^{u+r} (\Phi_s^* f)(x) ds - \int_0^r (\Phi_s^* f)(x) ds] \quad (A2.9) \\ &= \lim_{u \rightarrow 0} u^{-1} [\int_r^{u+r} (\Phi_s^* f)(x) ds - \int_0^u (\Phi_s^* f)(x) ds]. \end{aligned}$$

Hence we perceive that

$$D_X \omega(f, r) = \Phi_r^* f(x) - f(x) = (\Phi_r^* - 1) f(x). \quad (A2.10)$$

We next demonstrate that $\omega(f, r) \in C^\infty(X, M)$ and that

$D_X^n \omega(f, r) = (\Phi_r^* - 1) D_X^{n-1} f$ by application of lemma 2.1. We have

$$D_X^n \omega(f, r) = D_X^{n-1} [(\Phi_r^* - 1) f] = (\Phi_r^* - 1) D_X^{n-1} f, \quad (\text{A2.11})$$

since $f \in C^\infty(M) \subset C^\infty(X, M)$, so that clearly, as was required $\omega(f, r) \in C^\infty(X, M)$.

To show that $\omega(f, r)$ is r -differentiable and that $d\omega(f, r)/dr = \Phi_r^* f$, it suffices to observe the equalities:

$$\begin{aligned} \frac{d\omega}{dr}(f, r) &= \lim_{u \rightarrow 0} u^{-1} [\int_0^{r+u} (\Phi_s^* f)(x) ds - \int_0^r (\Phi_s^* f)(x) ds] \\ &= \lim_{u \rightarrow 0} u^{-1} \int_r^{r+u} (\Phi_s^* f)(x) ds = \Phi_r^* f(x). \end{aligned} \quad (\text{A2.12})$$

Finally, consider $\Phi_s^* \omega(f, r)$; we have the following sequence of equalities:

$$\begin{aligned} \Phi_s^* \omega(f, r) &= \Phi_s^* \int_0^r (\Phi_t^* f)(x) dt = \int_0^r (\Phi_{s+t}^* f)(x) dt = \int_s^{r+s} (\Phi_t^* f)(x) dt \\ &= \int_0^{r+s} (\Phi_t^* f)(x) dt - \int_0^s (\Phi_t^* f)(x) dt = \omega(f, r+s) - \omega(f, s). \end{aligned} \quad (\text{A2.13})$$

This result concludes the proof of the lemma.

We now describe the group of unitary transformations of $\mathcal{L}_\rho^2(M)$ whose infinitesimal generator corresponds to the observable $Q(P+f)$.

Theorem 2.3: A one-parameter group of unitary transformations on $\mathcal{L}_\rho^2(M)$.

Let P be a complete momentum of M generating a C^∞ vector field X , and let f be a C^∞ function on M . Define the class of operators

$U_t: \mathcal{L}_\rho^2(M) \rightarrow \mathcal{L}_\rho^2(M)$, $t \in \mathbb{R}$, by the prescription

$$U_t \psi = (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \exp \frac{i}{\hbar} \omega(f, t) \Phi_t^* \psi; \quad (\text{A2.14})$$

then the set $\{U_t | t \in \mathbb{R}\}$ comprises a one-parameter group of unitary transformations.

Proof: We first show that, for each $t \in \mathbb{R}$, U_t is unitary; that is

$$\forall \phi, \psi \in \mathcal{L}^2_\rho(M) \quad (U_t \psi, U_t \phi) = (\psi, \phi) , \quad (\text{A2.15})$$

by means of the equalities

$$(U_t \psi, U_t \phi) = \int_M (U_t \psi)^* (U_t \phi) \rho = \int_M \phi_t^* (\psi^* \phi \rho) = \int_M \psi^* \phi \rho = (\psi, \phi) , \quad (\text{A2.16})$$

where the former integrals exist since the last does.

Turning now to the group structure of $\{U_t | t \in \mathbb{R}\}$ we need

only show that $U_t \circ U_s = U_{t+s}$, this latter being established as follows:

$$\begin{aligned} U_t \circ U_s &= (\phi_t^* \rho / \rho)^{\frac{1}{2}} \exp \frac{i}{\hbar} \omega(f, t) \phi_t^* [(\phi_s^* \rho / \rho)^{\frac{1}{2}} \exp \frac{i}{\hbar} \omega(f, s) \phi_s^*] \quad (\text{A2.17}) \\ &= (\phi_{t+s}^* \rho / \rho)^{\frac{1}{2}} \exp \frac{i}{\hbar} \omega(f, t) \exp \frac{i}{\hbar} (\omega(f, t+s) - \omega(f, t)) \phi_{t+s}^* \\ &= U_{t+s} , \end{aligned}$$

in which sequence we have applied part [3] of lemma 2.1.

The existence of the self-adjoint operator $Q(P+f)$ satisfying the equation

$$U_t = \exp \frac{i}{\hbar} Q(P+f)t ,$$

is now assured by Stone's theorem^(a5), so that it remains only to exhibit the form of $Q(P+f)$. Thus restricting attention to the set of $C_0^\infty(M)$ functions we deduce

Theorem 2.4: On the symmetric restriction of $Q(P+f)$.

The operator $Q(P+f)$ when restricted to the $C_0^\infty(M)$ functions has the differential expression

$$Q_0(P+f) = -i\hbar(X + \frac{1}{2} \operatorname{div} X + if/\hbar) , \quad (\text{A2.18})$$

is symmetric, and satisfies the formal quantization rule

$$Q_0(P+f) = Q_0(P) + Q_0(f) . \quad (\text{A2.19})$$

Proof: We have that

$$\frac{d}{dt} U_t \psi \Big|_{t=0} = \frac{i}{\hbar} Q(P+f) , \quad (A2.20)$$

and hence, restricting our attention to $\psi \in C_0^\infty(M)$,
we have by explicit calculation

$$\frac{d}{dt} U_t \psi \Big|_{t=0} = \frac{d}{dt} \left[\left(\frac{\phi_t^*}{\rho} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} \omega(f,t)} \phi_t^* \psi \right] = \left(X + \frac{1}{2} \operatorname{div} X + \frac{if}{\hbar} \right) \psi , \quad (A2.21)$$

which is the desired result, the formal quantization axiom being clearly satisfied, and the symmetry of $Q_0(P+f)$ following from the denseness of the domain $C_0^\infty(M)$.

Moreover we may show, by applying an analysis similar to that of appendix 1 of chapter 1, that $Q_0(P+f)$ is essentially self-adjoint whenever P is complete. We require firstly some technical results.

Lemma 2.4: Let Ω be an (unbounded) self-adjoint operator on a Hilbert space \mathcal{H} ; let D_0 , a subset of the domain of Ω , be a dense linear subspace of \mathcal{H} , and suppose that $U_t = \exp i\Omega t$, the unitary one-parameter group associated with Ω , leaves D_0 invariant. Then the restriction Ω_0 of Ω to D_0 is essentially self-adjoint.

Proof: see Abraham and Marsden^(a6).

Lemma 2.5: The symmetric extension of $Q_0(P+f)$ defined by

$$\Omega = -i\hbar(D_X + \frac{1}{2} \operatorname{div} X + i\hbar^{-1} f) , \quad (A2.22)$$

on the domain

$$D\Omega = \{ \psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C_0^\infty(X,M), \Omega\psi \in \mathcal{L}_\rho^2(M) \} , \quad (A2.23)$$

is essentially self-adjoint.

Proof: That Ω defines a symmetric restriction of $Q(P+f)$.

The set of $C_0^\infty(X, M)$ of infinitely X -differentiable functions of compact support is a linear subspace dense in $\mathcal{L}_\rho^2(M)$, so that, by lemma 2.4, we need only demonstrate that

$$U_t C_0^\infty(X, M) = C_0^\infty(X, M), \quad \forall t \in \mathbb{R}. \quad (A2.24)$$

This last is immediate from the definition of U_t ; for we have

$$\forall \psi \in C_0^\infty(X, M) \quad U_t \psi = (\Phi_t^* \rho / \rho)^{\frac{1}{2}} e^{\frac{i}{\hbar} \omega(f, t)} \Phi_t^* \psi, \quad (A2.25)$$

and that $(\Phi_t^* \rho / \rho)^{\frac{1}{2}} \in C_0^\infty(M) \subset C_0^\infty(X, M)$, $\omega(f, t) \in C_0^\infty(X, M)$ by part [2] of lemma 2.2, and $\Phi_t^* \psi \in C_0^\infty(X, M)$ also by lemma 2.2 part [1], so that finally $U_t \psi \in C_0^\infty(X, M)$. Thus $\forall \psi \in C_0^\infty(X, M)$, $U_t \psi \in C_0^\infty(X, M)$ and (A2.24) follows from the unitary character of U_t .

Lemma 2.6: The closure $Q_0^{\dagger\dagger}(P+f)$ of the above defined operator $Q_0(P+f)$, and the operator Ω of lemma 2.5 satisfy the inclusion relation

$$Q_0^{\dagger\dagger}(P+f) \supseteq \Omega. \quad (A2.26)$$

Proof: Since P is a complete C^∞ momentum, $Q_0(P)$ is essentially self-adjoint, by theorem 1 of chapter 1, and hence by theorem 2 of chapter 1, $C_0^\infty(X, M) \subset DQ(P) = DQ_0^{\dagger\dagger}(P)$. Thus by the definition of the closure of an operator^(a7), there exists at least one sequence $\{\psi_k \in C_0^\infty(M)\} \rightarrow \psi \in C_0^\infty(X, M)$ such that the corresponding sequence $\{Q_0(P)\psi_k\} \rightarrow Q_0^{\dagger\dagger}(P)\psi$. Moreover, since $\psi \in C_0^\infty(X, M)$, then, $\forall f \in C_0^\infty(M)$, $f\psi \in \mathcal{L}_\rho^2(M)$, and hence $\{f\psi_k\} \rightarrow f\psi$. Finally collecting these terms we have shown that

$$\forall \psi \in C_0^\infty(X, M) \exists \{\psi_k \in C_0^\infty(M)\} \rightarrow \psi: \{(Q_0(P) + f)\psi_k\} \rightarrow Q_0^{\dagger\dagger}(P)\psi + f\psi,$$

and noting that $(Q_0^{\dagger\dagger}(P) + f)\psi = \Omega\psi$, we infer the desired result.

We may now state the third of our principal results.

Theorem 2.7: On the essential self-adjointness of $Q_0(P+f)$.

If P is a complete momentum, and f a C^∞ function on M , then the operator $Q_0(P+f)$ is essentially self-adjoint.

Proof: We have that, by lemma 2.5, Ω is essentially self-adjoint, and, by lemma 2.6, that $\Omega \subset Q_0^{\dagger\dagger}(P+f)$; hence $Q_0^{\dagger\dagger}(P+f)$ is essentially self-adjoint and thus symbolically

$$\overline{Q_0^{\dagger\dagger}(P+f)} = (Q_0^{\dagger\dagger}(P+f))^{\dagger} = Q_0^{\dagger\dagger\dagger}(P+f), \quad (\text{A2.27})$$

but now $Q_0^{\dagger\dagger}(P+f) = \overline{Q_0}(P+f)$ is closed, as is $Q_0^{\dagger}(P+f)$, so that^(a8)

$$\overline{Q_0^{\dagger\dagger}(P+f)} = \overline{Q_0}(P+f), \text{ and } Q_0^{\dagger\dagger\dagger}(P+f) = Q_0^{\dagger}(P+f), \quad (\text{A2.28})$$

and hence $Q_0(P+f)$ is essentially self-adjoint as required.

We now turn our attention to the converse proposition the proof being a natural generalisation of a similar proof for the case $f = \text{div } X = 0$ given in Abraham and Marsden^(a9). We first state two results which we shall find necessary.

Lemma 2.8: Let $f(x, t)$, $g(x) = \int f(x, t) dt$ be functions in $L^2_\rho(M)$; then

$$\int \|f(x, t)\| dt \geq \| \int f(x, t) dt \|, \quad (\text{A2.29})$$

in which $\|f\| = (\int f^* f \rho)^{\frac{1}{2}}$ is the norm induced by the scalar product on $L^2_\rho(M)$.

Proof: This follows from the defⁿ of the (Riemann) integral, and the Cauchy-Schwartz inequality.

Lemma 2.9: The symmetric operator Ω_0 is essentially self-adjoint if and only if the integral equations

$$\forall \phi \in D\Omega_0 \quad (\psi, (\Omega_0 \pm i\hbar E)\phi) = 0 \quad (\text{A2.30})$$

imply that $\psi = 0$.

Proof: see Hellwig^(a10).

We may now state the fourth of our results.

Theorem 2.10: On the dequantization of a quantum observable linear in momentum.

Let Ω be a self-adjoint operator on $\mathcal{L}^2_\rho(M)$ possessing an essentially self-adjoint restriction Ω_0 defined by the differential expression

$$\Omega_0 = -i\hbar(X + \frac{1}{2} \operatorname{div} X + i\hbar^{-1}f), \quad (\text{A2.31})$$

on the domain

$$D\Omega_0 = \{\psi \in \mathcal{L}^2_\rho(M) \mid \psi \in C^\infty_0(M), \Omega_0 \psi \in \mathcal{L}^2_\rho(M)\}. \quad (\text{A2.32})$$

Then the associated vector field X generated by Ω_0 is complete except for a set of measure zero.

Proof: It suffices by lemma 2.9 to demonstrate that if the vector field X is not complete¹, then there exists a non-zero vector $\psi(x) \in \mathcal{L}^2_\rho(M)$ such that

$$\forall \phi \in D\Omega_0 \quad (\psi, (\Omega_0 - i\hbar)\phi) = 0; \quad (\text{A2.33})$$

for then $(\Omega_0 - i\hbar)D\Omega_0$ is not dense in $\mathcal{L}^2_\rho(M)$, and hence Ω_0 is not essentially self-adjoint.

¹By "complete" is here intended complete else on a set of measure zero.

Let us therefore elect ex hypotheso that X is a C^∞ incomplete vector field, and assume that there exists a set E of finite (non-zero) measure such that, say², if ϕ_t is the local flow generated by X , then $\phi_t(x)$ fails to be defined for sufficiently large positive values of t whenever $x \in E$. Introduce further the subsets E_τ of E defined as the sets of points of E for which $\phi_t(x)$, $x \in E_\tau$ fails to be defined for all $t \geq \tau > 0$, so that we have the equality

$$E = \bigcup_{\tau=1}^{\infty} E_\tau. \quad (A2.34)$$

Next observe that at least one such E_τ , $E_\tau = A$ say, must be of non-zero measure; for the union of sets of measure zero is itself of measure zero. It is with this such particularly chosen set A that we shall subsequently be concerned. We complete the preliminaries by extending the definition of the pull-backs ϕ_t^* of ϕ_t , onto functions and onto the density ρ induced by the Riemannian structure on M , by means of the auxiliary functions F_t^* themselves defined as

$$F_t^* = \begin{cases} \phi_t^*, & \text{whenever } \phi_t^* \text{ is well-defined,} \\ 0, & \text{otherwise.} \end{cases} \quad (A2.35)$$

We are now able to introduce a function $\psi(x) \neq 0$ satisfying (A2.33) and to prescribe this function by the integral

$$\psi(x) = \int_{-\infty}^{+\infty} dt e^{-t} \left(\frac{F_t^* \rho}{\rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,t)} F_t^* \chi(A), \quad (A2.36)$$

² If this condition is not satisfied then consider that P becomes $-P$, and f , $-f$, in the sequel.

in which $\chi(A)$ is the characteristic function of A ; and $\omega(f, t)$ is the auxiliary function defined as in (A2.4) of lemma 2.2 with $F_t^* f(x)$ replacing $\Phi_t^* f(x)$ in the integrand.

We show sequentially that $\psi(x)$ defines a vector of $L^2_\rho(M)$ such as is sufficient to satisfy (A2.33)

[1] $\psi(x)$ prescribed by the integral (A2.36)

defines a function on M . It suffices to show that the integrand is non-zero only for a finite range of variable of integration, a result which we demonstrate in several steps.

(i) If x lies on a complete maximal integral curve of x then necessarily $\Phi_t(x) \notin A \quad \forall t \in \mathbb{R}$ and hence $F_t^* \chi(A)(x) = 0$, so that $\psi(x) = 0$ identically.

(ii) If x lies on an incomplete maximal integral curve such that $\Phi_t(x) \in M \quad \forall t \in \mathbb{R}^+$ then again necessarily $\Phi_t(x) \notin A \quad \forall t \in \mathbb{R}^+$ and hence $F_t^* \chi(A)(x) = 0, \quad t > 0$.

(iii) If x lies on an incomplete maximal integral curve then

$F_t^* \chi(A) = 0, \quad t < -\tau$. For let

$t = -\tau + \epsilon$, so that $\Phi_\tau(\Phi_{-\tau-\epsilon}(x)) =$

$\Phi_{-\epsilon}(x)$, which for sufficient small

ϵ is defined, so that $\Phi_{-\tau-\epsilon}(x) \notin A$

and hence $F_t^* \chi(A) = 0, \quad t < -\tau$.

Hence collecting these results we see that the integration has a lower limit $-\tau$ and a finite upper limit determined by the necessarily finite, upper limit of the t -range, or symbolically,

$$\psi(x) = \int_{-\tau}^{\phi(x) < \infty} dt e^{-t} (F_t^* \rho / \rho)^{\frac{1}{2}} e^{i\omega(f,t)} F_t^* \chi(A) . \quad (A2.37)$$

This completes this stage of the proof.

[2] $\psi(x)$ is an element of $\mathcal{L}_{\rho}^2(M)$.

We have by lemma 2.8 that if $\| \cdot \|$ denotes the norm $(\cdot, \cdot)^{\frac{1}{2}}$ on $\mathcal{L}_{\rho}^2(M)$, then

$$\|\psi(x)\| \leq \int_{-\infty}^{+\infty} e^{-t} \| (F_t^* \rho / \rho)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,t)} F_t^* \chi(A) \| dt , \quad (A2.38)$$

and immediately from the properties of the norm

$$\|\psi(x)\| \leq \int_{-\infty}^{+\infty} e^{-t} \| (F_t^* \rho / \rho)^{\frac{1}{2}} F_t^* \chi(A) \| dt . \quad (A2.39)$$

Consider now the action of the operator

$(F_t^* \rho / \rho)^{\frac{1}{2}} F_t^*$: we have either $F_t^* = 0$ or else $F_t^* = \Phi_t^*$ when $(F_t^* \rho / \rho)^{\frac{1}{2}} F_t^* = (\Phi_t^* \rho / \rho)^{\frac{1}{2}} \Phi_t^*$ is the unitary

operator of (A2.15) of theorem 2.3 with $f = 0$,

and hence is measure-preserving. Thus we

perceive that

$$\| (F_t^* \rho / \rho)^{\frac{1}{2}} F_t^* \chi(A) \| \leq \| \chi(A) \| , \quad (A2.40)$$

and hence finally that

$$\|\psi(x)\| \leq \| \chi(A) \| \int_{-\tau}^{\infty} e^{-t} dt = e^{\tau} \| \chi(A) \| , \quad (A2.41)$$

as required.

[3] The function $\psi(x)$ satisfies the technical property

$$(F_s^* \rho / \rho)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s)} F_s^* \psi(x) = e^s \psi(x), \quad (A2.42)$$

provided that s is sufficiently small.

This is the result of an explicit calculation under the assumption that $F_s^* = \Phi_s^*$. We have the following equalities

$$\begin{aligned} & \left(\frac{\Phi_s^* \rho}{\rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s)} \Phi_s^* \left[e^{-t} \left(\frac{\Phi_t^* \rho}{\rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,t)} \Phi_t^* \right] \\ &= \left(\frac{\Phi_s^* \rho}{\rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s)} e^{-t} \left(\frac{\Phi_s^* \circ \Phi_t^* \rho}{\Phi_s^* \rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s+t) - \frac{i\omega}{\hbar}(f,s)} \Phi_s^* \circ \Phi_t^* \\ &= e^{-t} \left(\frac{\Phi_{s+t}^* \rho}{\rho} \right)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s+t)} \Phi_{s+t}^*, \end{aligned} \quad (A2.43)$$

in which we have assumed that both $\Phi_s^* \circ \Phi_t^*$ and Φ_{s+t}^* exist. If either exists then both do, and Φ_ϵ^* exists for sufficiently small ϵ , so that it follows that

$$(F_s^* \rho / \rho)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,s)} F_s^* \psi(x) = e^s \psi(x), \quad (A2.44)$$

as was required.

$$[4] \forall \phi \in C_0^\infty(M) \quad (\psi, (X + \frac{1}{2} \operatorname{div} X + if + 1)\phi) = 0. \quad (A2.45)$$

We have, setting $U_t = (F_t^* \rho / \rho)^{\frac{1}{2}} e^{\frac{i\omega}{\hbar}(f,t)} F_t^*$, that

$$(\psi, (X + \frac{1}{2} \operatorname{div} X + if)\phi) = \lim_{t \rightarrow 0} \int_M \psi^* \frac{U_t \phi - \phi}{t}, \quad (A2.46)$$

as follows from an analysis parallel to that of theorem 2.4, and that, for sufficiently small t ,

$\psi^* = U_t \circ U_{-t} \psi^*$, so that substituting we deduce

$$(\psi, (X + \frac{1}{2} \operatorname{div} X + if)\phi) = \lim_{t \rightarrow 0} t^{-1} \left[\int_M (U_t (U_{-t} \psi))^* U_t \phi - \int_M \psi^* \phi \right], \quad (A2.47)$$

but U_t is measure-preserving for sufficiently small t , hence

$$\begin{aligned} (\psi, (X + \frac{1}{2} \operatorname{div} X + if)\phi) &= \lim_{t \rightarrow 0} t^{-1} \left[\int_M (U_{-t} \psi)^* \phi - \psi^* \phi \right] \quad (\text{A2.48}) \\ &= \lim_{t \rightarrow 0} t^{-1} \int_M (e^{-t} - 1) \psi^* \phi = - \int_M \psi^* \phi = -(\psi, \phi). \end{aligned}$$

Thus we have demonstrated the required result.

The only remaining kernel result of this section is the explicit determination of the self-adjoint operator $Q(P+f)$ when P is a complete momentum. This is furnished by our fifth theorem.

Theorem 2.11: On the quantum observable generated by the observable $P+f$.

If P is a C^∞ complete momentum and f is a C^∞ function on M , then $Q(P+f)$ exists, and moreover $Q(P+f) = Q(P) + Q(f)$.

Proof: The proof of this result is exactly parallel to that of the form of $Q(P)$ in appendix 2 of chapter 1.

Turning now our attention to the special properties which obtain when $D_X^{-1}f$ defines an element of $C^1(X, M)$ such that $D_X(D_X^{-1}f) = f$, we have the following:

Theorem 2.12: Some special forms when $f = D_X g$.

When the function $\omega(f, t)$ assumes the form

$$\omega(f, t) = (\Phi_t^* - 1)g(f), \quad (\text{A2.49})$$

that is when there exists a function $g(f) \in C^1(X, M)$: $D_X g = f$, then the following equations hold between the unitary, self-adjoint, and spectral functions generated by the symmetric forms $Q_0(P)$ and $Q_0(P+f)$:

$$U_t^{Q(P+f)} = e^{+ig/\hbar} U_t^{Q(P)} e^{-ig/\hbar} ; \quad (A2.50)$$

$$Q(P+f) = e^{+ig/\hbar} Q(P) e^{-ig/\hbar} ; \quad (A2.51)$$

$$E_\lambda^{Q(P+f)} = e^{+ig/\hbar} E_\lambda^{Q(P)} e^{-ig/\hbar} . \quad (A2.52)$$

Proof: We first show that when $g(f) \in C^1(X, M)$ exists, then $\omega(f, t)$ assumes the form (A2.49). We have that $\omega(f, t)$ has the properties

$$\omega(f, 0) = 0, \quad d\omega(f, t)/dt = (\Phi_t^* - 1)f , \quad (A2.53)$$

by lemma 2.2, that $(\Phi_t^* - 1)g(f) = 0$ when $t = 0$, and finally that

$$\frac{d}{dt}(\Phi_t^* - 1)g = \lim_{s \rightarrow 0} s^{-1} (\Phi_{s+t}^* g - \Phi_t^* g) = \Phi_t^* \lim_{s \rightarrow 0} s^{-1} (\Phi_s^* g - g) = \Phi_t^* f , \quad (A2.54)$$

whence the result follows.

Substituting the expression (A2.49) into the definition (A2.15) of $U_t^{Q(P+f)}$ we immediately deduce (A2.50), and hence by differentiation at $t = 0$, or else by direct calculation (A2.51). The result (A2.52) then follows by observing that $e^{ig/\hbar}$ is independent of the spectral parameter λ .

Appendix 3: On the algebraic quantization of observables linear in momentum.

[1] Theorem 11: On the Lie algebra of observables linear in momentum.

Proof: The defined bracket is clearly both bilinear and anti-symmetric, so that the only non-trivial demonstration is that of the Jacobi identity, this last being readily obtained by explicit calculation.

[2] Theorem 12: On the Lie algebra of formal quantum observables linear in momentum.

Proof: It suffices to prove that $Q_0(\{P_1+f_1, P_2+f_2\}) = \{Q_0(P_1+f_1), Q_0(P_2+f_2)\}$. We have that, by definition,

$$\{Q_0(P_1+f_1), Q_0(P_2+f_2)\} = -i\hbar([X_1, X_2] + \frac{1}{2} \text{div}[X_1, X_2] + \frac{i}{\hbar}(X_1 f_2 - X_2 f_1))$$

$= Q_0(\{P_1+f_1, P_2+f_2\})$ as required, all the other results being trivial.

[3] Theorem 13: The basic laws of quantization for observables linear in momentum.

Proof: These results follow analogously to those of [4] of appendix 1.

[4] Theorem 14: Some particular Lie subalgebras of $P+F$.

Proof: All but part [14] follow from the observation that if A is a subalgebra of P within P_C , then $A+F$ is a subalgebra of $P+F$ within P_C+F . The remaining part is trivial.

References to the Appendices
of Chapter 2

References to the Appendices
of Chapter 2

- a1: Loomis L.H. and Sternberg S.: "Advanced Calculus", Addison Wesley (1968), §13.3, pp515-516.
- a2: Bishop R.L. and Crittenden R.J.: "Geometry of Manifolds", Academic Press (1964), §2.4, example (1), p.26.
- a3: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978) p.99, exercise 2.2G.
- a4: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), p.70, corollary 2.1.19.
- a5: Prugovecki E.: "Quantum Mechanics in Hilbert Space", Academic Press (1971), p.335, theorem 6.1.
- a6: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), p.141, lemma 2.6.13.
- a7: Akhiezer N.I. and Glazman I.M.: "Theory of Linear Operators in Hilbert Space", volume 1, Frederick Ungar (1961), §38, pp78-79.
- a8: Naimark M.A.: "Linear Differential Operators", part II, George G. Harrap (1968), §4, p.12.
- a9: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978), pp142-143, theorem 2.6.15.
- a10: Hellwig G.: "Differential Operators of Mathematical Physics", Addison-Wesley (1967), pp180-181, theorems 2 and 3.

Chapter 3

"The Quantization of Multilinear Momentum Observables"

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§1: Introduction and Résumé.

We develop in this, the third and final chapter, some aspects of the problem of the quantization of the multilinear momentum observables, and begin our discussion with a definition:

- [1] An observable A is a multilinear momentum observable (multilinear momentum) of order n if and only if, in every chart (U, α) of the cotangent bundle T^*M of a Riemannian manifold (M, G) , A has, relative to the coordinate system $\{(x^i, p_i) | i \in [1, m]\}$, the tensor form¹

$$A = a^{i_1 \dots i_n}_{(x^k)} p_{i_1} \dots p_{i_n}, \quad n \in \mathbb{N} \cup \{0\}, \quad (1)$$

in which $a^{i_1 \dots i_n}_{(x^k)}$ is a fully symmetric contravariant tensor⁽¹⁾ of order n .

Besides being the natural generalisations of the (linear) momenta $a^i_{p_i}$, these, the multilinear momentum observables, are of interest and significance for the following reasons:

- [2] they include not only the free Hamiltonian but also most, or perhaps all, of the naturally occurring (scalar) observables of dynamics, and
- [3] a large number of classical observables have, in terms of the multilinear momenta, a Taylor series decomposition

$$A = \sum_{k=0}^{\infty} a^{i_1 \dots i_k}_{(x^k)} p_{i_1} \dots p_{i_k}, \quad (2)$$

¹For the interpretation of the right hand expression of the equality (1) when $n = 0$, as well as for all subsequent implicit notational conventions in this chapter, the reader is referred to appendix 1.

which, together with the assumption of linearity

$$Q_0(a^{i_1 \dots i_k} p_{i_1} \dots p_{i_k} + b^{i_1 \dots i_\ell} p_{i_1} \dots p_{i_\ell}) = \\ Q_0(a^{i_1 \dots i_k} p_{i_1} \dots p_{i_k}) + Q_0(b^{i_1 \dots i_\ell} p_{i_1} \dots p_{i_\ell}) \quad (3)$$

permits their quantization in terms of the quantum observables $Q_0(a^{i_1 \dots i_n} p_{i_1} \dots p_{i_n})$.

Having defined the multilinear momenta and briefly motivated their study, we should ideally now seek to implement the programme of quantization as outlined in the second chapter; specifically we should

- [4] identify the symmetric differential operator $Q_0(A)$ generated naturally by the observable A and defined upon the dense set $C_0^\infty(M)$, and
- [5] ascertain whether a given observable A is quantizable by testing $Q_0(A)$ for essential self-adjointness, and finally determine explicitly the quantum observable $Q(A) = Q_0^\dagger(A)$ whenever this test is met.

It is, however, immediately clear that such a programme could not, in the case of the multilinear momenta, be carried out either to completion or with full rigour; for in the case of [4] no suitable and generally agreed physical or mathematical principle is known which will determine $Q_0(A)$, and in the case of [5] the mathematical difficulties involved in the analytic manipulation, as is required, of n^{th} order partial differential operators are all but insuperable. It is thus perhaps not surprising that there seems to have been no previous systematic and rigorous discussion of the quantization of the multilinear momenta, although much work has been carried out, more especially into the problems surrounding the bilinear momenta and the Hamiltonian⁽²⁻⁸⁾.

We shall, therefore, be more modest than previously in our goals, both in system and in rigour, and shall limit ourselves in the sequel to the following problems;

- [6] the determination of the most general form of symmetric differential operator $Q_0(A)$, so as to delimit the degree of uncertainty in the form of $Q_0(A)$ which needs be resolved by some further mathematical or physical principle,
- [7] the discussion, especially in the case of the bilinear momenta, of some possible means of prescribing a unique differential expression for $Q_0(A)$,
- [8] the study of some of the conditions required for the quantizability of local classical observables derived from the multilinear observable A , local observables being chosen so as to allow the development of essential self-adjointness boundary conditions which do not, in general, exist for global observables, and finally,
- [9] the exemplification of some of the features of our discussion by means of an explicitly worked special case.

It is to these problems and their inter-relations that we address ourselves in this chapter.

§2: On the General Form of the Symmetric Operators $Q_0(A)$.

Our task in this section will be the determination of the most general admissible form of the differential expression of the symmetric operator $Q_0(A)$ of formal quantization, generated by the

(classical) multilinear momentum observable $A = a^{i_1 \dots i_n} p_{i_1} \dots p_{i_n}$.

To this end let us introduce a set of three axioms which, while clearly necessary, are not sufficient for the unique determination of $Q_0(A)$, but which nevertheless yield much information as to its general form, and insight into the degree of "reasonable uncertainty" in the quantization of multilinear momentum observables.

These axioms, which will require no detailed justification here, are as follows:

[10] $Q_0(A)$ has a differential expression given in terms of the coordinates $\{x^i | i \in [1, m]\}$ by the partial differential operator

$$Q_0(A) = (-i\hbar)^n \sum_{k=0}^n \eta^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k}, \quad (4)$$

in which the coefficients $\eta^{i_1 \dots i_k}(x)$ are fully symmetric in all indices and are assumed to be real valued, and in which in particular the leading term is prescribed by

$$\eta^{i_1 \dots i_n}(x^k) = a^{i_1 \dots i_n}(x^k), \quad (5)$$

as is in accordance with the formal prescription

$$Q_0(p_i) = -i\hbar(\partial_i + \frac{1}{2} \operatorname{div}(\frac{\partial}{\partial x^i})) . \quad (6)$$

[11] $Q_0(A)\psi$, $\forall \psi \in C_0^\infty(M)$ transforms as an invariant⁽⁹⁾, as does the wave-function ψ itself.

[12] $Q_0(A)$ is a symmetric operator defined on the domain $C_0^\infty(M)$.

The immediate consequence of these axioms is the following proposition, which is the starting point of our subsequent discussion.

Theorem 1: On the differential expression of $Q_0(A)$.

Let $A = a^{i_1 \dots i_n} p_{i_1} \dots p_{i_n}$ denote an observable multilinear in momentum, in which $a^{i_1 \dots i_n}(x^k)$ is a fully symmetric contravariant tensor of order n . Then the differential expression of any admissible symmetric operator, which is consistent with the axioms [10]-[12] above, assumes the general form

$$Q_0(A) = \sum_{k=0}^n (-i\hbar)^n b^{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k}, \quad (7)$$

where $b^{i_1 \dots i_k}(x^\ell)$ is a fully symmetric contravariant tensor of order k , and δ_{i_ℓ} denotes the action of the covariant derivative (10) with respect to x^{i_ℓ} . Moreover the tensors $b^{i_1 \dots i_k}(x^\ell)$ satisfy the "initial condition"

$$b^{i_1 \dots i_n} = a^{i_1 \dots i_n}, \quad (8)$$

and the recurrence relation

$$b^{i_1 \dots i_\ell} = \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} b^{i_1 \dots i_k}_{|i_{\ell+1} \dots i_k}, \quad \ell \in [0, n], \quad n \in \mathbb{N}, \quad (9)$$

in which $\binom{k}{\ell}$ denotes the binomial coefficient defined as

$$\binom{k}{\ell} = \begin{cases} k! / [\ell! (k-\ell)!], & k \geq \ell, \\ 0, & k < \ell, \end{cases} \quad (10)$$

and in which the vertical bar denotes covariant differentiation.

Proof: see appendix 2, the index notation being as in appendix 1.

We may illustrate the content of the recurrence (9) by taking the example of a multilinear observable of order 4, $a^{ijkl} p_i p_j p_k p_l$, when the following equations are obtained:

$$b^{ijkl} = a^{ijkl}, \quad (11)$$

$$b^{ijk} = -b^{ijk} + 4b^{ijk\ell}_{|\ell},$$

$$b^{ij} = b^{ij} - 3b^{ijk}_{|k} + 6b^{ijk\ell}_{|k\ell},$$

$$b^i = -b^i + 2b^{ij}_{|j} - 3b^{ijk}_{|jk} + 4b^{ijk\ell}_{|jk\ell},$$

$$b = b - b^i_{|i} + b^{ij}_{|ij} - b^{ijk}_{|ijk} + b^{ijk\ell}_{|ijk\ell}.$$

We note that the tensors b^{ij} and b are undetermined, but that, when given some prescription for these, all the remaining tensors are specified uniquely by the above system (11).

A more general analysis shows that to prescribe a unique differential operator for $Q_0(A)$ it is necessary to specify explicitly, in addition to the quantity $b^{i_1 \dots i_n} = a^{i_1 \dots i_n}$, the tensors

$$b^{i_1 \dots i_{n-2k}}, \quad k \in [1, [n/2]], \quad (12)$$

in which $[n/2]$ denotes the integer part of $n/2$ ⁽¹¹⁾. We shall therefore, seek a "canonical" decomposition of $Q_0(A)$ into a sum of symmetric² operators $\Xi_0(B_{n-2k})$ each one of which is determined by the classical observable

$$B_{n-2k} = b^{i_1 \dots i_{n-2k}} p_{i_1} \dots p_{i_{n-2k}}, \quad k \in [1, [n/2]], \quad (13)$$

the operators Ξ_0 being introduced as follows:

[13] The auxiliary operator $\Xi_0(B)$, where $B = b^{i_1 \dots i_v} p_{i_1} \dots p_{i_v}$,

$v \in [0, n]$ is any multilinear momentum, is given explicitly

by the differential expression

$$\Xi_0(B) = (-i\hbar)^v \sum_{k=0}^v \alpha_k^v b^{i_1 \dots i_v}_{|i_{k+1} \dots i_v} \delta_{i_1} \dots \delta_{i_k}, \quad (14)$$

² The symmetry of these operators is demonstrated in appendix 2.

in which the coefficients α_k^v are any real numbers obeying the recurrence relationship

$$\alpha_\ell^v = \sum_{k=\ell}^v (-1)^{v+k} \binom{k}{\ell} \alpha_k^v, \quad (15)$$

and subject to the initial condition

$$\alpha_v^v = 1, \quad (16)$$

the domain of definition being simply

$$D\Xi_o(A) = \{\psi \in \mathcal{L}_o^2(M) \mid \psi \in C_o^\infty(M), \Xi_o(A)\psi \in \mathcal{L}_o^2(M)\}. \quad (17)$$

The canonical decomposition of $Q_o(A)$ can now be given.

Theorem 2: On the canonical decomposition of $Q_o(A)$.

The general symmetric operator $Q_o(A)$ as given in (7) has the canonical decomposition

$$Q_o(A) = \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} \Xi_o(B_{n-2k}), \quad (18)$$

so that the coefficients $b_{i_1 \dots i_\ell}$, $\ell \in [0, n]$, of the tensorial decomposition (7) become

$$b_{i_1 \dots i_\ell} = \sum_{k=0}^{[\frac{n-\ell}{2}]} \alpha_\ell^{n-2k} b_{i_1 \dots i_{n-2k} | i_{\ell+1} \dots i_{n-2k}}. \quad (19)$$

Proof: see appendix 2.

Note especially that the canonical decomposition given by (18) and (19) exists for every choice of the coefficients α_k^n satisfying the recurrence relation (15) and constraint (16). We leave open until §3 the question of which particular choice of α_k^n leads to the greatest simplification of the theory, and content ourselves for the present with the concrete choice determined by the conditions

$$\alpha_{n-2k}^n = 0, \quad k \in [1, [n/2]] . \quad (20)$$

This results in the following explicit forms;

$$\equiv_o(a^i_{p_i}) = (-i\hbar)(a^i_{\delta_i} + \frac{1}{2}a^i_{|i}) , \quad (21)$$

$$\equiv_o(a^{ij}_{p_i p_j}) = (-i\hbar)^2 (a^{ij}_{\delta_i \delta_j} + a^{ij}_{|j \delta_i}) ,$$

$$\equiv_o(a^{ijk}_{p_i p_j p_k}) = (-i\hbar)^3 (a^{ijk}_{\delta_i \delta_j \delta_k} + \frac{3}{2}a^{ijk}_{|k \delta_i \delta_j} - \frac{1}{4}a^{ijk}_{|ijk}) ,$$

so that by (18) we deduce;

$$Q_o(a^i_{p_i}) = (-i\hbar)(a^i_{\delta_i} + \frac{1}{2}a^i_{|i}) , \quad (22)$$

$$Q_o(a^{ij}_{p_i p_j}) = (-i\hbar)^2 (a^{ij}_{\delta_i \delta_j} + a^{ij}_{|j \delta_i} + c(a^{ij})) ,$$

$$Q_o(a^{ijk}_{p_i p_j p_k}) = (-i\hbar)^3 (a^{ijk}_{\delta_i \delta_j \delta_k} + \frac{3}{2}a^{ijk}_{|k \delta_i \delta_j} - \frac{1}{4}a^{ijk}_{|ijk}) \\ - \hbar^2 (-i\hbar)(b^k(a^{ijk})_{\delta_k} + \frac{1}{2}b^k_{|k}) ,$$

in which the quantities $c(a^{ij})$ and $b^k(a^{ijk})$ are undetermined tensors of the indicated type.

The canonical decomposition, as developed in theorem 2, and as embodied in the low-order examples (22), precisely circumscribes the degree of arbitrariness remaining in the differential expression of $Q_o(A)$. In particular we may observe

[14] that in the case of a momentum observable $a^i_{p_i}$ the form of $Q_o(a^i_{p_i})$ is completely determined by the axioms [10]-[12], so that the starting point of Mackey's scheme is consistent with the theory of this chapter, and

[15] that in the case of a bilinear momentum observable $a^{ij}_{p_i p_j}$ the form of $Q_o(a^{ij}_{p_i p_j})$ is determined else for an arbitrary function $c(a^{ij})$ which, as we shall

see³, does not effect the quantizability, in accordance with the criterion of essential self-adjointness proposed in chapter 2, of the observables $a^{ij} p_i p_j$.

The problem of the formal quantization of the multilinear momentum observables is thus reduced to the determination of the tensor quantities $B_{n-2k}(A)$, $k \in [1, [n/2]]$, a task which admits of no obvious or ready solution.

Before turning briefly to this task in §4, we first develop the problem of the essential self-adjointness of the general observables $Q_0(A)$, or more precisely, as this is mathematically simpler, of their local quantum representatives $Q_\Gamma^0(A)$, defined over a local set Γ of the manifold.

§3: On Local Quantum Observables corresponding to Multilinear Momentum Observables.

We develop in this section some aspects of the theory of the local quantization of the observables multilinear in momentum. Our analysis is essentially parallel to that of the discussion in §6.1 of chapter 1 on local momentum observables, but that, in the absence of any known criterion for the existence of the global quantum observables $Q(A) = Q_0^\dagger(A)$, we take as our formal local observable the operator

$$Q_\Gamma^0(A) = \pi Q_0(A) \pi, \quad (23)$$

in which Γ is any finite local set of regular boundary $\partial\Gamma$, and in which π is the projector onto Γ given by

$$\forall \psi \in \mathcal{L}_\rho^2(M) \quad \pi\psi(x) = \begin{cases} \psi(x), & x \in \Gamma \\ 0, & x \notin \Gamma. \end{cases} \quad (24)$$

³ This is demonstrated in §3.

This alternative definition of a local quantum observable has the merit that it may define for some Γ a self-adjoint closure $(\pi Q_0(A)\pi)^\dagger$ even when $Q(A)$ does not itself exist. We further assume, as a device to simplify our calculations,

[16] that the local set Γ is coverable by a single coordinate chart, in terms of the coordinates $\{x^i | i \in [1, m]\}$ of which we shall express the results and theorems of the sequel.

The starting point of our analysis is the following theorem:

Theorem 3: On the auxiliary operators $\Xi_\Gamma^\infty(B)$, and $Q_\Gamma^\infty(A)$.

Let $\Xi_\Gamma^\infty(B)$ denote for a general multilinear momentum observable the operator of differential expression

$$\Xi_\Gamma^\infty(B)\psi(x) = \begin{cases} (-i\hbar)^\nu \sum_{k=0}^{\nu} \alpha_k^{i_1 \dots i_\nu} b_{i_{k+1} \dots i_\nu} \delta_{i_1} \dots \delta_{i_k} \psi(x), & x \in \Gamma \\ 0 & , x \notin \Gamma, \end{cases} \quad (25)$$

and domain of definition

$$D\Xi_\Gamma^\infty(B) = \{\psi \in \mathcal{L}_\rho^2(M) | \psi \in C^\infty(\Gamma), \Xi_\Gamma^\infty(B)\psi \in \mathcal{L}_\rho^2(M)\} ; \quad (26)$$

and let $Q_\Gamma^\infty(A)$ be defined by the prescription

$$Q_\Gamma^\infty(A) = \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} \Xi_\Gamma^\infty(B_{n-2k}), \quad (27)$$

in which, as above, the quantities $B_{n-2k}(A)$ are the multilinear momentum observables

$$B_{n-2k}(A) = b^{i_1 \dots i_{n-2k}} p_{i_1} \dots p_{i_{n-2k}}. \quad (28)$$

Then the adjoint of the formal local quantum observable

$Q_\Gamma^0(A)$ satisfies the inclusion

$$(Q_\Gamma^0(A))^\dagger \supset Q_\Gamma^\infty(A), \quad (29)$$

and hence the operator $Q_{\Gamma}^0(A)$ is essentially self-adjoint only if the operator $Q_{\Gamma}^{\infty}(A)$ is symmetric.

Proof: see appendix 3.

Hence we immediately perceive that the conditions which assure the symmetry of the operators $Q_{\Gamma}^{\infty}(A)$ are necessary conditions for the essential self-adjointness of $Q_{\Gamma}^0(A)$. It is possible to explicitly determine these symmetry generated constraints which resolve themselves into integral conditions upon the boundary $\partial\Gamma$ of Γ in accordance with the following theorem.

Theorem 4: Boundary conditions on $\partial\Gamma$ equivalent to the symmetry of $Q_{\Gamma}^{\infty}(A)$.

The operator $\Xi_{\Gamma}^{\infty}(A)$ is symmetric if and only if the integral equations

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} \beta_{\rho k}^n \int_{\partial\Gamma} a_{i_1 \dots i_n}^{i_1 \dots i_n} \psi_{|i_{\rho+k+2} \dots i_n}^* |i_1 \dots i_{\rho} \phi_{|i_{\rho+1} \dots i_{\rho+k}} \hat{n}_{i_{\rho+k+1}} d\sigma = 0, \quad (30)$$

in which \hat{n}_i denotes the covariant components of the unit normal to the surface $\partial\Gamma$ at any point, are satisfied for all $\psi, \phi \in C^{\infty}(\Gamma)$, the coefficients $\beta_{\rho k}^n$ being given by the formula

$$\beta_{\rho k}^n = \sum_{\ell=\rho+k+1}^n \alpha_{\ell}^n (-1)^{\ell} \binom{\ell-1-k}{\rho}. \quad (31)$$

Moreover the operator $Q_{\Gamma}^{\infty}(A)$ is symmetric if and only if the integral equations

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} \int_{\partial\Gamma} y_{n\rho k}^{i_1 \dots i_{\rho+k+1}} \psi_{|i_1 \dots i_{\rho} \phi_{|i_{\rho+1} \dots i_{\rho+k}} \hat{n}_{i_{\rho+k+1}} d\sigma, \quad (32)$$

are satisfied identically for all $\psi, \phi \in C^{\infty}(\Gamma)$, the quantities $y_{n\rho k}^{i_1 \dots i_{\rho+k+1}}$ being fully symmetric tensors prescribed by the relation

$$y_{npk}^{i_1 \dots i_{\rho+k+1}} = \sum_{i=0}^{\lfloor \frac{n-1-k-\rho}{2} \rfloor} \beta_{\rho k}^{n-2i} b_{i_{\rho+k+2} \dots i_{n-2i}}^{i_1 \dots i_{n-2i}}. \quad (33)$$

Proof: see appendix 3.

We may exemplify the, somewhat inaccessible, integral conditions (32) above by quoting their explicit form when $n = 1$ and 2 , these cases corresponding to the (linear) momenta and the bilinear momenta. We have

$$\int_{\partial \Gamma} a_{\hat{n}_i}^{i_1} \psi^* \phi \, d\sigma = 0, \quad (34)$$

and

$$\int_{\partial \Gamma} a_{\hat{n}_i}^{ij} (\psi_{|j}^* \phi - \psi^* \phi_{|j}) \, d\sigma = 0. \quad (35)$$

Two observations regarding the above surface integrals are in order: Firstly

[17] that (34) is reducible⁽¹²⁾ to the simple condition,

$$a_{\hat{n}_i}^{i_1}(x) = 0, \text{ almost everywhere in } \partial \Gamma, \quad (36)$$

which, for a regular boundary $\partial \Gamma$ and a C^∞ vector field $X = a_{\hat{n}_i}^{i_1} / \partial x^{i_1}$, assures the invariance of Γ under the flow ϕ_t of X , this last being precisely the (necessary and sufficient) condition for the existence of a local momentum observable $Q_\Gamma(A)$ derived in §6.1 of the first chapter;

and secondly

[18] that the symmetry of $Q_\Gamma^\infty(a_{p_i p_j}^{ij})$ is independent of the particular choice of the (undetermined) function $c(a^{ij})$ of (22), and therefore the question of whether the formal observable $Q_\Gamma^0(A)$ is essentially self-adjoint can be answered in the negative without prior

knowledge of the quantity $c(a^{ij})$.

To further simplify the relationships (31)-(33) it is necessary to introduce a definite known form for the observables $\Xi_o(A)$ or equivalently to specify a particular set of coefficients α_k^n , $k \in [0, n]$; specifically we shall, in the sequel, elect the following:

[19] In the sequel the operators $\Xi_o(B)$ are to be taken as

defined by the differential expressions

$$\Xi_o(B) = \begin{cases} (-i\hbar)^{2v} \delta_{i_1} \dots \delta_{i_v} b^{i_1 \dots i_{2v}} \delta_{i_{v+1}} \dots \delta_{i_{2v}}, & \text{even case,} \\ (-i\hbar)^{2v+1} \delta_{i_1} \dots \delta_{i_v} \frac{1}{2} [\delta_{i_{v+1}} b^{i_1 \dots i_{2v+1}}]_+ \delta_{i_{v+2}} \dots \delta_{i_{2v+1}}, & \text{odd case,} \end{cases} \quad (39)$$

in which $[,]_+$ denotes the anticommutator bracket of operators, the symmetry of $\Xi_o(B)$ being strongly suggested by their visual form.

This choice of $\Xi_o(A)$ results in the following values for the coefficients α_k^n and $\beta_{\rho k}^n$.

Theorem 5: On the explicit expressions of the coefficients α_k^n and $\beta_{\rho k}^n$:

The quantities α_k^v determined by the operators $\Xi_o(B)$ of [19] in accordance with the prescription [13]

$$\Xi_o(B) = (-i\hbar)^v \sum_{k=0}^v \alpha_k^v b^{i_1 \dots i_v} \delta_{i_{k+1} \dots i_v} \delta_{i_1} \dots \delta_{i_k}, \quad (38)$$

are given by

$$\alpha_\ell^{v=2m} = \binom{m}{\ell-m}, \quad \ell \in [0, v], \quad (39)$$

$$\alpha_\ell^{v=2m+1} = \binom{m+1}{\ell-m} - \frac{1}{2} \binom{m}{\ell-m}, \quad \ell \in [0, v]; \quad (40)$$

and the corresponding quantities $\beta_{\rho k}^n$ of (31) have the explicit

form

$$\beta_{\rho k}^{v=2m} = \begin{cases} (-1)^\rho \binom{m-\rho-1}{k-m} , & \rho < m, m \leq k , \\ -(-1)^k \binom{m-k-1}{\rho-m} , & k < m, m \leq \rho , \end{cases} \quad (41)$$

$$\beta_{\rho k}^{v=2m+1} = \begin{cases} (-1)^\rho \left[\binom{m-\rho}{k-m} - \frac{1}{2} \binom{m-\rho-1}{k-m} \right] , & \rho < m, m \leq k , \\ (-1)^k \left[\binom{m-k}{\rho-m} - \frac{1}{2} \binom{m-k-1}{\rho-m} \right] , & k < m, m \leq \rho , \end{cases} \quad (42)$$

all the undefined coefficients being identically zero.

Proof: see appendix 3.

A list of the lowest order coefficients α_k^n and $\beta_{\rho k}^n$ is given in table 1 overleaf.

The above rather technical results enable a reduction of the symmetry induced boundary conditions on $Q_\Gamma^\infty(A)$ to a form whose only unknowns are the primary undetermined quantities $B_{n-2k}(A)$, $k \in [0, [n/2]]$. These conditions are by theorem 3 necessary, and in the special case of $A = a^i p_i$ sufficient, for the essential self-adjointness of $Q_\Gamma^0(A)$. To bring the analyses of this section into perspective, and to enable the deduction of two striking theorems, we shall make the following, highly plausible if rather sweeping, conjecture:

[20] The symmetry of $Q_\Gamma^\infty(A)$ is both necessary and sufficient⁴
for the essential self-adjointness of $Q_\Gamma^0(A)$.

The force of this conjecture is sufficient to enable deductions to be made concerning the existence of local quantum observables given the formally accessible symmetry boundary conditions on $Q_\Gamma^\infty(A)$; indeed

⁴We admit as a priori admissible quantities $B_{n-2k}(A)$ determining $Q_\Gamma^0(A)$ only, say, those whose associated tensors $b_{1 \dots i_{n-2k}}^i$ are infinitely differentiable.

Table 1: A List of the Lowest Order Coefficients a_k^n and $\beta_{\rho k}^n$

a_k^n	k=0	k=1	k=2	k=3	k=4	k=5	k=6	k=7	k=8	k=9
n=1	$\frac{1}{2}$	1	0	0	0	0	0	0	0	0
n=2	0	1	1	0	0	0	0	0	0	0
n=3	0	$\frac{1}{2}$	$\frac{3}{2}$	1	0	0	0	0	0	0
n=4	0	0	1	2	1	0	0	0	0	0
n=5	0	0	$\frac{1}{2}$	2	$\frac{5}{2}$	1	0	0	0	0
n=6	0	0	0	1	3	3	1	0	0	0
n=7	0	0	0	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{9}{2}$	$\frac{7}{2}$	1	0	0
n=8	0	0	0	0	1	4	6	4	1	0
n=9	0	0	0	0	$\frac{1}{2}$	3	7	8	$\frac{9}{2}$	1
n=10	0	0	0	0	0	1	5	10	10	5

The quantities $\beta_{\rho k}^n$ are represented in the form of matrices $B^{(n)}$, the coefficients $\beta_{\rho k}^n$ being the entry in the $\rho+1^{\text{st}}$ row and $k+1^{\text{st}}$ column of the matrix $B^{(n)}$.

$$B^{(1)} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}; \quad B^{(2)} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \quad B^{(3)} = \begin{bmatrix} 0 & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix};$$

$$B^{(4)} = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad B^{(5)} = \begin{bmatrix} 0 & 0 & \frac{1}{2} & \frac{3}{2} & 1 & 0 \\ 0 & 0 & -\frac{1}{2} & -1 & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 & 0 & 0 & 0 \\ \frac{3}{2} & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

armed with this conjecture we may immediately deduce the following key proposition.

Theorem 6: Sufficient conditions for the quantizability of the local observables $Q_\Gamma^O(A)$.

The boundary conditions

$$y_{npk}^{i_1 \dots i_{p+k+1}} \hat{n}_{i_1} (\partial \Gamma) = 0, \quad (43)$$

or, as is equivalent the constraints

$$a_{i_1 \dots i_p}^{i_1 \dots i_n} \hat{n}_{i_{p+1}} (\partial \Gamma) = 0, \quad 0 \leq p \leq [n/2 - \frac{1}{4}], \quad (44)$$

$$b_{i_1 \dots i_p}^{i_1 \dots i_{n-2\sigma}} \hat{n}_{i_{p+1}} (\partial \Gamma) = 0, \quad 0 \leq p \leq [n/2 - \frac{1}{4}] - \sigma, \quad 1 \leq \sigma \leq [n/2 - \frac{1}{4}], \quad (45)$$

are sufficient that the observables $Q_\Gamma^O(A)$ be essentially self-adjoint.

Proof: Subject to the above conjecture: see appendix 3.

Note that the boundary conditions of theorem 6 are not, in general, necessary; as can be seen by noting that the quantum observable $[Q_\Gamma^O(a^i_{p_i})]^3$ is essentially self-adjoint, that is, does satisfy the boundary conditions (32), provided only that $a^i \hat{n}_i (\partial \Gamma) = 0$, whereas this latter condition does not assure that $a^{ijk} = a^i a^j a^k$ satisfies the boundary conditions (44). Nevertheless we have, in the particular case of a one-dimensional manifold the following stronger result:

Theorem 7: Necessary and sufficient conditions for the quantizability on a one-dimensional manifold of the local observable $Q_\Gamma^O(A)$.

The boundary conditions (44) and (45) of the above theorem 6, which become for a one-dimensional manifold $(M, G) = (\mathcal{R}, \sqrt{g})$ with $\Gamma = (a, b)$, simply

$$b_{i_1 \dots i_{n-2\sigma}}^{i_1 \dots i_{n-2\sigma}}(a) = b_{i_1 \dots i_{\rho}}^{i_1 \dots i_{n-2\sigma}}(b) = 0, \quad (46)$$

$$0 \leq \rho \leq [n/2 - \frac{1}{2}] - \sigma, \quad 0 \leq \sigma \leq [n/2 - \frac{1}{2}],$$

are both necessary and sufficient that $Q_{(a,b)}^0(A)$ be essentially self-adjoint.

Proof: sufficiency is subject to the above conjecture: see appendix 3.

The significance of the above two theorems consists in their reduction of the analytic, and therefore inaccessible, question of the essential self-adjointness of a formal local observable $Q_{\Gamma}^0(A)$ to the question of whether a group of algebraic conditions are satisfied by the component tensors $B_{n-2k}(A)$, $k \in [0, [n/2]]$, on the boundary of the corresponding local set Γ . Thus, given as locally quantizable a particular class of multilinear observables A , we may delimit, at least to some extent, the admissible forms of the quantities $B_{n-2k}(A)$; or alternatively, given the quantities $B_{n-2k}(A)$ and a local set Γ , we may determine a subclass of the locally quantizable observables A .

§4: On the Determination of the Tensor Quantities $B_{n-2k}(A)$, $k \in [0, [n/2]]$.

Having determined the general admissible form of the quantum observables $Q_0(A)$ corresponding to a multilinear momentum observable A , and having ascertained the conditions determining the existence of local quantum observables $Q_{\Gamma}(A)$, we now enquire whether any systematic procedure can be adopted such as will uniquely determine the quantities $B_{n-2k}(A)$, or, equivalently, such as will prescribe the unique form of the formal observable $Q_0(A)$. We find it convenient to divide our discussion into two parts; the first, more detailed, concerned with the special case of the bilinear observable $a^{ij}_{p_i p_j}$, and the second, rather brief and speculative, concerned with the general case of the multilinear observable $a^{i_1 \dots i_n}_{p_{i_1} \dots p_{i_n}}$.

54.1: On the determination of the formal quantum operator $Q_o(a^{ij}_{p_i p_j})$.

Turning now to the unique specification of the formal quantum observable $Q_o(a^{ij}_{p_i p_j})$ having the general form

$$Q_o(a^{ij}_{p_i p_j}) = (-i\hbar)^2 (a^{ij}_{\delta_i \delta_j} + a^{ij}_{|j \delta_i} + c(a^{ij})) , \quad (47)$$

we here outline and briefly contrast three distinct procedures which determine the unknown and real valued function $c(a^{ij})$.

We begin our discussion of the first of these procedures by stating the following axiom of quantization:

[21] The operation of formal quantization is such that the observables which are constants of classical free motion have as quantum analogues constants of free quantum motion, or symbolically

$$Q_o(\{a^{ij}_{p_i p_j}, g^{ij}_{p_i p_j}\}) = (+i\hbar)^{-1} [Q_o(a^{ij}_{p_i p_j}), Q_o(g^{ij}_{p_i p_j})], \quad (48)$$

in which $\{ , \}$ denotes the Poisson bracket, $[,]$ the commutator bracket, and g^{ij} the contravariant metric tensor of the configuration space.

This axiom has, as have similar and more general such axioms, been studied by Bloore et alia⁽¹³⁻¹⁶⁾, who have, in a series of papers, obtained the following results:

[22] The assumption of linearity (3), together with conservation under quantization of the constants of free motion, yields for the conserved bilinear momenta the expression

$$c(a^{ij}) = \frac{1}{4} a^{i|j}_{i|j} = \frac{1}{4} g^{jk} a^{i}_{i|jk} , \quad (49)$$

as may alternatively be demonstrated from axiom [21] assuming in place of linearity that the free quantum Hamiltonian $Q_o(g^{ij}_{p_i p_j})$ is simply, as in Mackey's scheme,

the Laplacian, this latter result being demonstrated in appendix 4.

[23] If the expression (49) is then held to obtain for all second order multilinear momenta, then we may deduce by direct calculation that it is incompatible with the Dirac⁽¹⁷⁾ correspondence

$$Q_o(\{a^{ij}_{p_i p_j}, b^k_{p_k}\}) = (+i\hbar)^{-1} [Q_o(a^{ij}_{p_i p_j}), Q_o(b^k_{p_k})], \quad (50)$$

the correspondence being admissible if and only if the momentum $b^k_{p_k}$ is Killing.

An alternative procedure for the specification of the scalar function $c(a^{ij})$, at least for a subclass, of the bilinear momenta is the "squaring axiom":

[24] The formal quantization of a bilinear momentum which is the square of a momentum is in accordance with the rule⁽¹⁸⁾

$$Q_o(b^i b^j_{p_i p_j}) = Q_o^2(b^i_{p_i}). \quad (51)$$

In view of the very natural character of this axiom it is perhaps surprising that it has as consequence that

[25] the squaring axiom is inconsistent with the linearity property for the observables $Q_o(a^{ij}_{p_i p_j})$,

a result demonstrated by counterexample in appendix 4.

As a final method of quantization we propose the following:

[26] The formal quantum operators $Q_o(a^{ij}_{p_i p_j})$ are such that $c(a^{ij})$ has the linear form

$$c(a^{ij}) = \alpha a^{i|j}_{i|j} + \beta a^{ij}_{|ij}, \quad (52)$$

in which α and β are real constants, and moreover satisfy the requirement that each positive definite classical observable $a^{ij} p_i p_j$ results upon quantization in a positive definite differential operator.

This results, after substituting from examples (appendix 4), in the ideally simple form

$$c(a^{ij}) = 0 . \quad (53)$$

Turning now to compare the above modes of quantization, we immediately perceive that, whereas each procedure is based upon a natural correspondence, each is nevertheless inconsistent with all the others. There would seem, at present, to be no overwhelming reason to prefer any one of the above procedures to any other. However, so as to be definite in the sequel, we shall assume that the choice [26] is the correct one, since this results in the ideally simple canonical decomposition

$$Q_o(a^{ij} p_i p_j) = \equiv_o(a^{ij} p_i p_j) , \quad (54)$$

and, as has been demonstrated by Kimura⁽¹⁸⁾, in the attractive equivalent expression

$$Q_o(a^{ij} p_i p_j) = g^{-\frac{1}{2}} Q_o(p_i) g^{\frac{1}{2}} a^{ij} g^{\frac{1}{2}} Q_o(p_j) g^{-\frac{1}{2}} . \quad (55)$$

in which as usual g denotes the determinant of the metric tensor g_{ij} .

§4.2: Some remarks upon the general problem of determining the quantities $B_{n-2k}(A)$, $k \in [0, [n/2]]$.

Let us address the problem of determining in the general case the quantities $B_{n-2k}(A)$. We shall outline two possible methods of solution, discuss their limitations and advantages, and finally tentatively find in favour of the second means of quantization.

Consider firstly the following general axiom:

[27] The formal quantum operators $Q_0(A)$ corresponding to the multilinear momenta A are such that

$$Q_0(\{g^{ij}_{p_i p_j}, A\}) = (+i\hbar)^{-1} [Q_0(g^{ij}_{p_i p_j}), Q_0(A)] . \quad (56)$$

Whilst this is a natural and physically appealing quantization rule, it is nevertheless, as was demonstrated by Bloore, Assimakopoulos, and Ghobrial⁽²⁰⁾, in general inconsistent, the only cases when the above system (56) uniquely determines the operators $Q_0(A)$ (of at most second order) corresponding to reducible configuration manifolds, either of one-dimension, or of vanishing Ricci tensor, or of constant curvature. We may conclude, therefore, that this schema cannot have any general applicability in the problem of the quantization of multilinear momentum observables.

We may alternatively be less ambitious in our aims and demand instead that the system (56) above be valid only for those multilinear momenta which are constants of the free motion. The disadvantage of this reduced scheme lies in the extreme computational difficulty involved in the explicit calculation even of the lowest order observables $Q_0(A)$.

Restricting for the moment our attention to one-dimensional manifolds, we propose as our second axiom of quantization the following:

[28] The formal quantization of the multilinear momenta is such that the class of quantizable momenta is, in a sense to be made explicit below, "maximally large", the quantities

$B_{n-2k}(A)$ being assumed to have the general form

$$B_{n-2k}(A) = \epsilon_{2k}^n \frac{i_1 \dots i_n}{i_{n-2k+1} \dots i_n}, \quad k \in [0, [n/2]] , \quad (57)$$

in which the quantities ϵ_{2k}^n are real constants.

Recalling the necessary and sufficient conditions for the quantizability of a general local observable $Q_\Gamma^0(A)$ of theorem 7, and substituting the expressions (57) thereinto, we deduce, for the local quantizability of the observable A on the interval $\Gamma = (a,b)$, the conditions

$$\epsilon_{2k}^n a_{i_1 \dots i_n}^{i_1 \dots i_n} (c) = 0, \quad c \in \{a,b\}, \quad p \in [0, [n/2-1]] . \quad (58)$$

These may be illustrated for the special case of $n=5$, say, by the explicit system

$$\begin{aligned} a^{11111}(c) &= 0, & \epsilon_2^5 a_{11}^{11111}(c) &= 0, & \epsilon_4^5 a_{11111}^{11111}(c) &= 0, \\ a_{11}^{11111}(c) &= 0, & \epsilon_2^5 a_{1111}^{11111}(c) &= 0, \\ a_{11}^{11111}(c) &= 0, \end{aligned} \quad (59)$$

in which $c \in \{a,b\}$ and where we have noted, in accordance with (8), that $\epsilon_0^n = 1$. It is now immediate from the general pattern illustrated in (59) above, and the general independence of the various derivative conditions above, that, independent of the choice of Γ , the number of equations of constraint will be minimum provided only that

$$\epsilon_{2k}^n = 0, \quad k \in [0, [n/2-1]] . \quad (60)$$

This set of equations uniquely determines the observables of odd order, and determines the even ordered observables to within a scalar function $\epsilon_n^a i_1 \dots i_n$. Preservation of positivity under quantization ([25]) is then sufficient⁵ to set $\epsilon_n^n = 0$, so that, in the case of a one-dimensional manifold, [28] leads to the quantization rule

$$Q_0(A) = \Xi_0(A) . \quad (61)$$

⁵We omit the demonstration which is achieved by means of examples on the manifold $(M,G) = (\mathbb{R},1)$.

It is now natural to suppose, at least for the purpose of the sequel, that the above equation (61) holds quite generally for all manifolds, and all multilinear momentum observables. Indeed we conjecture, though cannot prove, that this generalisation is a consequence of axiom [28] above.

It will be well to note in closing that the above discussion of possible means of quantization does not claim to be exhaustive; for example we have not, due to technical problems in effecting a general comparison, included mention of Weyl's rule⁽²¹⁻²²⁾ or its generalisations, though this is in fact (for see footnote 6) inconsistent with the methods of quantization [24] and [26] above.

§5: An Illustration of the Proposed Quantization Scheme.

We develop in this section, by way of an illustration of the above proposed quantization scheme, the explicit form of certain quantum observables defined on the configuration manifold \mathcal{R} of coordinatization $\{x|x \in \mathcal{R}\}$ and with the usual metric. More precisely we shall, for a representative selection of C^∞ real-valued functions f of the (complete) momentum xp , seek to determine the coefficients α_k^f of the expansion

$$Q_0(f(xp)) = \sum_{k=0}^{\infty} \alpha_k^f Q_0^k(xp) , \quad (62)$$

in accordance with the requirements,

[29] that the Taylor series decomposition of $f(xp)$ enables the reduction of the quantization problem to that of the observables $Q_0(x^k p^k)$ by means of the axiom

$$Q_0(f(xp)) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} Q_0(x^k p^k) , \quad (63)$$

and

[30] that the quantization of the component observables

$Q_o(x^k p^k)$ is prescribed by the equations

$$Q_o(x^k p^k) = \equiv_o(x^k p^k) . \quad (64)$$

Let us, therefore, seek a decomposition of the operators $Q_o(x^k p^k)$ in terms of the powers of the fundamental quantum momentum $Q_o(xp)$, so as to obtain the following theorem:

Theorem 8: On the expansion of the operators $Q_o(x^k p^k)$, $k \in N$.

The operators $Q_o(x^k p^k)$ have a decomposition of the form

$$Q_o(x^k p^k) = \sum_{j=0}^k (-i\hbar)^{k-j} \beta_j^k Q_o^j(xp) , \quad (65)$$

the coefficients β_j^k of which are prescribed by the system

$$\beta_j^{2\ell} = \beta_{j+1}^{2\ell+1} = \sum_{i=j}^{2\ell} S_{2\ell}^i \binom{i}{j} (\ell - \frac{1}{2})^{i-j} , \quad \ell \in Nu\{o\}, j \in [o, 2\ell] , \quad (66)$$

in which S_j^i denote Stirling numbers of the first kind⁽²³⁾,

and in particular satisfy the conditions

$$\beta_{2j+1}^{2\ell} = \beta_{2j}^{2\ell-1} = 0, \quad \ell \in N, j \in [o, \ell] . \quad (67)$$

Proof: see appendix 5.

Hence we may by explicit calculation from (66) deduce the explicit decompositions⁶;

$$\begin{aligned} Q_o(x^2 p^2) &= Q_o^2(xp) + \frac{1}{4} \hbar^2 , \\ Q_o(x^3 p^3) &= Q_o^3(xp) + \frac{1}{4} \hbar^2 Q_o(xp) , \end{aligned} \quad (68)$$

⁶We remark in passing that the equation for $Q_o(x^2 p^2)$ shows, as is readily verified from the work of Castellani⁽²⁴⁾, that our proposed quantization scheme differs from and is inconsistent with Weyl's rule, the "symmetrization" rule, and the Born-Jordan rule.

$$Q_0(x^4 p^4) = Q_0^4(xp) + \frac{5}{2} \hbar^2 Q_0^2(xp) + \frac{9}{16} \hbar^4 ,$$

$$Q_0(x^5 p^5) = Q_0^5(xp) + \frac{5}{2} \hbar^2 Q_0^3(xp) + \frac{9}{16} \hbar^4 Q_0(xp) ,$$

$$Q_0(x^6 p^6) = Q_0^6(xp) + \frac{35}{4} \hbar^2 Q_0^4(xp) + \frac{259}{16} \hbar^4 Q_0^2(xp) + \frac{125}{64} \hbar^6 .$$

Consider now the effect of the following sequence of actions upon the system:

[31] Prepare the system in an eigenstate of the momentum $Q_0(xp)$,

so that, say,

$$Q_0(xp)\psi_\mu = \mu\psi_\mu, \quad \mu \in \mathcal{R}^+u\{0\} . \quad (69)$$

[32] Measure the observable $Q_0(x^k p^k)$ to obtain the (definite) value

$$\lambda = \sum_{j=0}^k (-i\hbar)^{k-j} \beta_j^k \mu^j . \quad (70)$$

Then the value of λ will, in general, differ from the classically expected value of μ^k , so that a measure of the departure from the classical result, or from a quantization scheme based upon the "power-law", $Q_0(x^k p^k) = Q_0^k(xp)$, can be obtained by plotting, in suitably normalised coordinates in figure 6 overleaf, the quantity $(\mu - \lambda^{1/k})/\hbar$ against μ/\hbar .

To conclude this section we state, in the form of a theorem, some further results which may be obtained by application of theorem 8 and the axiom [29] above.

Theorem 9: On the natural decompositions of some transcendental functions of the momentum xp .

The formal quantum operators; $Q_0(\sin xp)$, $Q_0(\cos xp)$, and their hyperbolic equivalents; $Q_0(\sinh xp)$, $Q_0(\cosh xp)$ have, in terms

Figure 6: To illustrate the distinction between the operators $Q_0^n(xp)$ and $Q_0(x^n p^n)$ as is in accordance with the proposed scheme of quantization.

For explanation of the diagrams refer to the associated text and note that $\Delta\mu = \mu^{-\lambda^{1/3}}$.

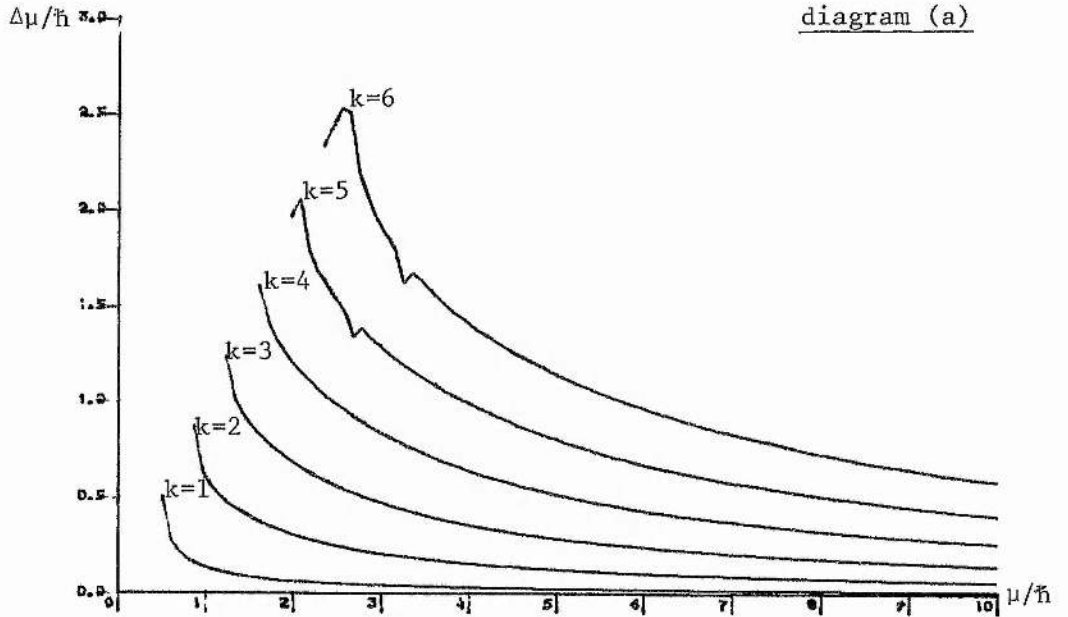


Diagram (a) shows the resultant arcs when $\Delta\mu/\hbar$ is plotted against μ/\hbar for the case of the even order observables $Q_0(x^{2k} p^{2k})$, $k \in [1,6]$.

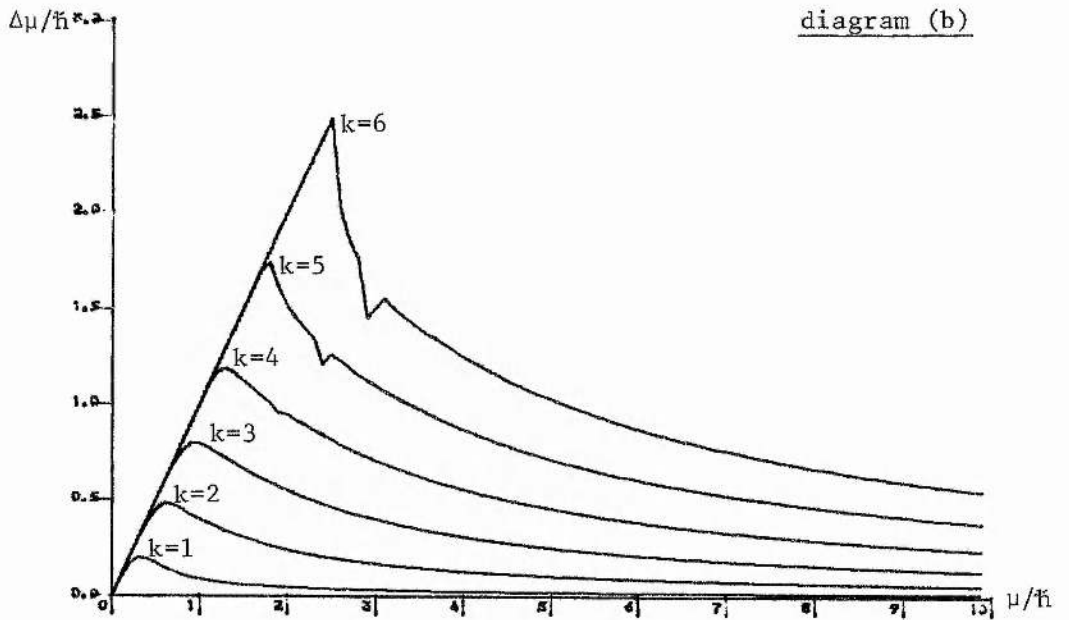


Diagram (b) shows the corresponding arcs when $\Delta\mu/\hbar$ is plotted against μ/\hbar for the case of the odd order observables $Q_0(x^{2k-1} p^{2k-1})$, $k \in [1,6]$.

of $Q_0(xp)$ the natural decompositions:

$$Q_0(\sin xp) = \sin(2/\hbar \sinh^{-1}(\hbar/2)Q_0(xp)) , \quad (71)$$

$$Q_0(\cos xp) = (1 + \hbar^2/4)^{-\frac{1}{2}} \cos(2/\hbar \sinh^{-1}(\hbar/2)Q_0(xp)) ,$$

$$Q_0(\sinh xp) = \sinh(2/\hbar \sin^{-1}(\hbar/2)Q_0(xp)) ,$$

$$Q_0(\cosh xp) = (1 + \hbar^2/4)^{-\frac{1}{2}} \cosh(2/\hbar \sin^{-1}(\hbar/2)Q_0(xp)) .$$

Proof: see appendix 5.

§6: Conclusion and Prospect.

The analyses of the foregoing sections have, in some measure, illuminated the problem of the quantization of the multilinear momentum observables, and have in particular led to a plausible and systematic scheme of (formal) quantization capable of wide application. Progress has been made regarding the essential self-adjointness of local quantum observables $Q_I^O(A)$, and conditions have been identified⁷ sufficient for their quantization. Finally the preferred scheme of quantization has been, by way of illustration, applied to the manifold $(\mathbb{R}, 1)$ and the observables $f(xp)$, functions of the complete momentum xp , and has led to rather pleasing explicit expressions for the quantum analogues of $\sin xp$ and $\cos xp$.

It is nevertheless immediately clear that the work of this chapter is far from exhaustive of the possibilities inherent in this field, and that a great breadth and depth of material remains unexplored in our brief survey. Among the many possible extensions we list only a few, whose development is suggested by analogy with the known results and procedures of the preceeding chapters. These are as follows:

⁷Subject to the conjecture [20].

- [33] the determination of the most general symmetric quantum operators $Q_0(\underline{A})$ corresponding to the class of non-scalar observables

$$\underline{A} = a^{i_1 \dots i_n} p_{i_1} \dots p_{i_n}, \quad n, m \in \mathbb{N} \setminus \{0\}, \quad n \neq m, \quad (72)$$

so as in particular to enable the formal quantization of such naturally occurring observables as the linear and angular momenta, and the Lenz vector⁽²⁵⁾;

- [34] an investigation into the global geometric properties of the bilinear tensors whose coordinate representation is the collection $a^{ij}(x^k)$ associated with the bilinear momentum $A = a^{ij} p_i p_j$, so as to discover whether any geometric property of a^{ij} can be correlated with the essential self-adjointness of any or all of the formal quantization operators $Q_0(A)$, and finally

- [35] the development, initially for the bilinear momenta, of a theory of measurement analogous to that set out in chapter 1, so as in particular to establish whether there obtains, between the essential self-adjointness of a formal quantum observable $Q_0(A)$, and some suitable concept of classical or quantum global measurability, a relationship which will permit the construction of a physically based axiom of quantizability.

It is our belief that the work of this chapter, more especially when augmented with the above proposed study, will provide a basic framework within which a detailed theory of the quantization of the multilinear momenta may ultimately be developed.

References to Chapter 3

References

- 1: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry...", second edition, Wiley (1964), §27, p.69, §40, p.97.
- 2: Bloore F.J., Assimakopoulos M., and Ghobrial I.R.: "Quantization as a deformation theory", J. Math. Phys. 17 (1976), 1034-1038.
- 3: Bloore F.J. and Routh L.: "The Covariant Form for Quantum-Mechanical Operators which are Quadratic in Momentum", Nuovo Cimento 47B (1978), 78-84.
- 4: Bloore F.J.: "Quantization on a Riemannian Manifold", Colloques Internationaux C.N.R.S., no.237, pp299-303.
- 5: Castellani L.: "Quantization Rules and Dirac's Correspondence", Nuovo Cimento 48A (1978), 359-363.
- 6: Underhill J. and Taraviras S.: "Weyl Quantization on a Sphere", Lecture Notes in Physics 50, Group Theoretical Methods in Physics, Fourth International Colloquium, Nijmegen 1975, Springer-Verlag (1976), pp210-216.
- 7: Wan K.K. and Viazminsky C.: "Lie algebra and the quantization of the Hamiltonian", J. Phys. A: Math. Gen. 12 (1979), 643-647.
- 8: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977), 1030-1044.
- 9: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry..." second edition, Wiley (1964), §18, p.51.
- 10: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry..." second edition, Wiley (1964), §33, pp81-84.
- 11: Hunter J. and Monk D.: "Algebra and Number Systems", Blackie/Chambers (1971), pp88-89.
- 12: Weinstock R.: "Calculus of Variations", McGraw-Hill (1952), pp16-17.
- 13: Bloore F.J. and Ghobrial I.R.: "Quantum mechanical ordering problem for observables which are linear in momentum", J. Phys. A: Math. Gen. 8 (1975), 1863-.

- 14: Bloore F.J. and Routh L.: "The Covariant Form for Quantum-Mechanical Operators which are Quadratic in Momentum", *Nuovo Cimento* 25B (1975), 78-84.
- 15: Bloore F.J., Assimakopoulos M., and Ghobrial I.R.: "Quantization as a deformation theory", *J. Math. Phys.* 17 (1976), 1034-1038.
- 16: Bloore F.J.: "Quantization on a Riemannian Manifold", *Colloques Internationaux C.N.R.S.*, no.237, pp299-303.
- 17: Dirac P.A.M.: "Principles of Quantum Mechanics", Oxford (1958), Chpt.4.
- 18: Temple G.: "The Fundamental Paradox of Quantum Theory", *Nature* (1935), 957.
- 19: Kimura T.: "On the Quantization of Non-Linear Theories", *Prog. Theor. Phys.* 46 (1971) 1261-1277.
- 20: Bloore F.J., Assimakopoulos M., and Ghobrial I.R.: "Quantization as a deformation theory", *J. Math. Phys.* 17 (1976), 1034-1038.
- 21: Weyl H.: "Theory of Groups and Quantum Mechanics", second edition, Dover (1931), p.275.
- 22: Underhill J. and Taraviras S.: "Weyl Quantization on a Sphere", *Lecture Notes in Physics* 50, Group Theoretical Methods in Physics, Fourth International Colloquium, Nijmegen 1975, Springer-Verlag (1976), pp210-216.
- 23: Jordan C.: "Calculus of Finite Differences", second edition, Chelsea Publishing Co. (1950), \$50, p.142.
- 24: Castellani L.: "Quantization Rules and Dirac's Correspondence", *Nuovo Cimento* 48A (1978), 359-368.
- 25: Schiff L.I.: "Quantum Mechanics", third edition, McGraw-Hill (1968), pp235-237.

Appendices to Chapter 3

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Appendix 1: Some Notational Conventions Implicit in Chapter 3.

This appendix comprises a group of naturally occurring notational conventions which are implicit in the manipulations of the following appendices and the text of chapter 3. Of these conventions perhaps only those of notes [6] and [7] will be novel to the reader.

[1] The usual summation and variable free-index conventions ^(a1) hold.

[2] The symbols "|" or "δ", each in context, denote the operation of covariant differentiation ^(a2) thus:

$$b_{|j_1 \dots j_\ell}^{i_1 \dots i_k}, k, \ell \in N, = \delta_{j_\ell} \dots \delta_{j_1} (b_{i_1 \dots i_k}) \quad (A1.1)$$

[3] The symbols "," and "∂" denote the operation of partial differentiation thus:

$$b_{,j_1 \dots j_\ell}^{i_1 \dots i_k}, k, \ell \in N, = \partial_{j_\ell} \dots \partial_{j_1} (b_{i_1 \dots i_k}) \quad (A1.2)$$

[4] The summation symbol $\sum_{k=\ell}^n$ has its usual meaning when $\ell \leq n$, but when $\ell > n$ the symbol represents a "null" sum thus:

$$\sum_{k=\ell}^n b_{i_1 \dots i_\ell}^{i_1 \dots i_k} = 0, \quad \ell > n. \quad (A1.3)$$

[5] The binomial coefficients $\binom{k}{\ell}$ have the augmented definition:

$$\binom{k}{\ell} = \begin{cases} k!/\ell!(k-\ell)! , & k \geq \ell , \quad k, \ell \geq 0 , \\ 0 & , \quad k < \ell , \quad k, \ell \leq 0 , \end{cases} \quad (A1.4)$$

and are undefined when $k < 0$ or $\ell < 0$.

[6] The symbol $a_{i_1 \dots i_n}^{i_1 \dots i_n}$ is to be interpreted, when

$n = 0$, as the (momentum independent) scalar function

$$a_{i_1 \dots i_0}^{i_1 \dots i_0} p_{i_1} \dots p_{i_0} = a(x^k).$$

[7] The following conventions apply as to the multiple index groupings.

(i) Increasing index symbols.

The increasing index symbol $i_{\ell+1} \dots i_k$, $k, \ell \in \mathbb{N} \cup \{0\}$, has the following interpretation:

if $k \geq \ell + 2$ then $i_{\ell+1} \dots i_k = (i_{\ell+1} \dots i_{k-1}) i_k$;

if $k = \ell + 1$ then $i_{\ell+1} \dots i_k = i_k$;

if $k = \ell$ then $i_{\ell+1} \dots i_k$ is void.

This is as illustrated by the explicit expressions below:

$$\sum_{k=0}^{n \geq 2} b_{i_1 \dots i_k} = b_{i_1 \dots i_n} + b_{i_1} + \sum_{k=2}^{n \geq 2} b_{i_1 \dots i_k}, \quad (A1.5)$$

and

$$\sum_{k=\ell \leq n}^{n \geq 2} b_{i_{k+1} \dots i_n} = \sum_{k=\ell}^{n-2} b_{i_{k+1} \dots i_n} + b_{i_n} + b_{i_1 \dots i_n}. \quad (A1.6)$$

(ii) Decreasing index symbols.

The decreasing index symbol $i_k \dots i_\ell$, $k, \ell \in \mathbb{N} \cup \{0\}$, has the following interpretation:

if $k > \ell$ then $i_k \dots i_\ell = i_k (i_{k-1} \dots i_\ell)$;

if $k = \ell$ then $i_k \dots i_\ell = i_k$;

if $k < \ell$ then $i_k \dots i_\ell$ is void.

This is as illustrated in the following example:

$$\sum_{k=0}^{n \geq 2} b_{i_k \dots i_1} = b_{i_1 \dots i_n} + b_{i_1} + \sum_{k=2}^n b_{i_k \dots i_1}. \quad (A1.7)$$

We note in conclusion that it will be obvious by context whether a given index group is increasing or decreasing.

This completes the first appendix.

Appendix 2: On the General Form of the Symmetric Operators $Q_0(A)$.

We develop in this appendix the form and canonical decomposition of the differential operator $Q_0(A)$ thereby demonstrating the theorems of §2 of chapter 3.

Lemma 2.1: On the tensorial representation of an invariant partial differential operator.

Any invariant partial differential expression of the form

$$\sum_{k=0}^n \eta^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k}, \quad (A2.1)$$

in which the coefficients $\eta^{i_1 \dots i_k}(x^\ell)$ may be chosen fully symmetric^(a3), may be reduced to a corresponding form involving only covariant differentiation, namely

$$\sum_{k=0}^n b^{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k}, \quad (A2.2)$$

in which the quantities $b^{i_1 \dots i_k}(x^\ell)$ are fully symmetric; the functions $b^{i_1 \dots i_k}$ being prescribed in terms of the decomposition

$$\partial_{i_1} \dots \partial_{i_k} = \delta_{i_1} \dots \delta_{i_k} + \sum_{\ell=0}^{k-1} \omega_{j_1 \dots j_\ell}^{i_1 \dots i_k} \partial_{j_1} \dots \partial_{j_\ell}, \quad (A2.3)$$

by the recurrence relation

$$b^{i_1 \dots i_k} = \sum_{\ell=k+1}^n b^{j_1 \dots j_\ell} \omega_{j_1 \dots j_\ell}^{i_1 \dots i_k} + \eta^{i_1 \dots i_k}, \quad \ell \leq n-1, \quad (A2.4)$$

and the initial condition

$$b^{i_1 \dots i_n} = \eta^{i_1 \dots i_n}. \quad (A2.5)$$

Proof: We demonstrate this result by direct substitution of (A2.3) and (A2.4) into the form (A2.2) to obtain the equalities;

$$\begin{aligned}
\sum_{k=0}^n b^{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k} &= \sum_{k=0}^n b^{i_1 \dots i_k} (\partial_{i_1} \dots \partial_{i_k} - \sum_{\ell=0}^{k-1} \omega_{i_1 \dots i_k}^{j_1 \dots j_\ell} \partial_{j_1} \dots \partial_{j_\ell}) \\
&\quad (A2.6) \\
&= \sum_{k=0}^n b^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k} - \sum_{\ell=0}^{n-1} \sum_{k=\ell+1}^n b^{i_1 \dots i_k} \omega_{i_1 \dots i_k}^{j_1 \dots j_\ell} \partial_{j_1} \dots \partial_{j_\ell} \\
&= \sum_{k=0}^n b^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k} - \sum_{\ell=0}^{n-1} (b^{i_1 \dots i_\ell} - \eta^{i_1 \dots i_\ell}) \partial_{i_1} \dots \partial_{i_\ell} \\
&= \sum_{k=0}^n \eta^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k} ;
\end{aligned}$$

and hence to deduce the required result. It will be sufficiently clear that $b^{i_1 \dots i_k}$ can be chosen fully symmetric.

Theorem 2.2: On the tensorial representation of the symmetric operator $Q_0(A)$.

The linear differential operator $Q_0(A)$ defined by the coordinate-based partial differential expression

$$Q_0(A) = (-i\hbar)^n \sum_{k=0}^n \eta^{i_1 \dots i_k} \partial_{i_1} \dots \partial_{i_k}, \quad (A2.7)$$

on the domain

$$DQ_0(A) = \{\psi \in \mathcal{L}_\rho^2(M) \mid \psi \in C_0^\infty(M), Q_0(A)\psi \in \mathcal{L}_\rho^2(M)\}, \quad (A2.8)$$

and satisfying the axioms [1]-[3] of chapter 3, has an equivalent tensor representation

$$Q_0(A) = (-i\hbar)^n \sum_{k=0}^n b^{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k}, \quad (A2.9)$$

in which the quantities $b^{i_1 \dots i_k}(x^\ell)$ are fully symmetric contravariant tensors of order k .

Proof: We observe, by lemma 2.1, that $Q_0(A)$ has an expression of the form (A2.9) where the quantities $b^{i_1 \dots i_k}(x^\ell)$ are fully

symmetric quantities but not, as yet, tensors. To demonstrate that they are indeed tensors of the indicated type, we transform the expression (A2.9) into its representation in terms of the coordinates $\{\bar{x}^i | i \in [1, m]\}$ and obtain

$$Q_0(A) = \sum_{k=0}^n (-i\hbar)^n \bar{b}^{i_1 \dots i_k} \bar{\delta}_{i_1} \dots \bar{\delta}_{i_k}, \quad (A2.10)$$

and hence, since $Q_0(A)\psi \quad \forall \psi \in DQ_0(A)$ is a tensor invariant,

$$\sum_{k=0}^n (\bar{b}^{i_1 \dots i_k} \frac{\partial x^{j_1}}{\partial \bar{x}^{i_1}} \dots \frac{\partial x^{j_k}}{\partial \bar{x}^{i_k}} - \bar{b}^{j_1 \dots j_k} \delta_{j_1} \dots \delta_{j_k}) = 0. \quad (A2.11)$$

Observe now that by axiom [1] of chapter 3 that

$$\bar{b}^{i_1 \dots i_n} = a^{i_1 \dots i_n}, \quad (A2.12)$$

where $a^{i_1 \dots i_n}$ is the fully symmetric contravariant tensor of order n induced by the multilinear momentum observable

$$A = a^{i_1 \dots i_n} p_{i_1} \dots p_{i_n}, \quad (A2.13)$$

so that the above sum becomes

$$(\bar{b}^{i_1 \dots i_{n-1}} \frac{\partial x^{j_1}}{\partial \bar{x}^{i_1}} \dots \frac{\partial x^{j_{n-1}}}{\partial \bar{x}^{i_{n-1}}} \partial_{j_1} \dots \partial_{j_{n-1}} + \text{lower order terms}) = 0.$$

Hence, since this statement is true for all wave functions

$\psi \in C_0^\infty(M)$, we have that the leading coefficient

$$\bar{b}^{i_1 \dots i_{n-1}} \frac{\partial x^{j_1}}{\partial \bar{x}^{i_1}} \dots \frac{\partial x^{j_{n-1}}}{\partial \bar{x}^{i_{n-1}}} - \bar{b}^{j_1 \dots j_{n-1}} = 0, \quad (A2.14)$$

and hence, by successive reduction of the order of the sum

(A2.11) that every $\bar{b}^{i_1 \dots i_k}$, $k \in [0, n]$ is a tensor of the specified type.

Lemma 2.3: For all states $\psi, \phi \in C_0^\infty(M)$, we have the identities,

$$\int_M b^{i_1 \dots i_k} \phi |_{i_1 \dots i_k} \psi^* = \int_M (-1)^k (b^{i_1 \dots i_k} \psi^*) |_{i_1 \dots i_k} \phi. \quad (A2.15)$$

Proof: Consider the identity

$$\begin{aligned} \int_M b^{i_1 \dots i_k} \phi |_{i_1 \dots i_k} \psi^* &= \int_M (b^{i_1 \dots i_k} \phi |_{i_1 \dots i_{k-1}} \psi^*) |_{i_k} \\ &\quad - \int_M (b^{i_1 \dots i_k} \psi^*) |_{i_k} \phi |_{i_1 \dots i_{k-1}}, \end{aligned} \quad (A2.16)$$

and apply, observing that ϕ and ψ are of compact support, the divergence theorem^(a4) to deduce

$$\int_M b^{i_1 \dots i_k} \phi |_{i_1 \dots i_k} \psi^* = (-1) \int_M (b^{i_1 \dots i_k} \psi^*) |_{i_k} \phi |_{i_1 \dots i_{k-1}}. \quad (A2.17)$$

Thus, by successive application of the above procedure, and by noting that $\phi |_{i_1 \dots i_k}, k \in [0, n]$, is of compact support, obtain that

$$\int_M b^{i_1 \dots i_k} \phi |_{i_1 \dots i_k} \psi^* = (-1)^k \int_M (b^{i_1 \dots i_k} \psi^*) |_{i_k i_{k-1} \dots i_1} \phi, \quad (A2.18)$$

the desired result then following from the symmetry of $b^{i_1 \dots i_k}$.

Lemma 2.4: For all $\psi \in C^\infty(M)$, we have the identities

$$(b^{i_1 \dots i_k} \psi) |_{i_1 \dots i_k} = \sum_{\ell=0}^k \binom{k}{\ell} b^{i_1 \dots i_k} |_{i_{\ell+1} \dots i_k} \psi |_{i_1 \dots i_\ell}. \quad (A2.19)$$

Proof: This is a fairly straightforward combinatorial problem depending upon the fully symmetric character of the tensors $b^{i_1 \dots i_k}$.

Theorem 2.5: On the constraints imposed by symmetry upon the tensors $b_{i_1 \dots i_k}$.

Axiom [3] of chapter 3 requires that the coefficients $b_{i_1 \dots i_k}^{(x^\ell)}$ of the differential expression

$$Q_0(A) = (-i\hbar)^n \sum_{k=0}^n b_{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k}, \quad (A2.20)$$

satisfy the recurrence relation

$$b_{i_1 \dots i_\ell} = \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} b_{i_{\ell+1} \dots i_k}^{i_1 \dots i_\ell}, \quad \ell \in [0, n \in \mathbb{N}]. \quad (A2.21)$$

Proof: We have by hypothesis that the symmetry condition

$$\forall \psi, \phi \in C_0^\infty(M) \quad \langle \psi | Q_0(A) | \phi \rangle = \langle Q_0(A) \psi | \phi \rangle, \quad (A2.22)$$

is identically satisfied, or as is equivalent that

$$\int_M ((-i\hbar)^n \sum_{k=0}^n b_{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k} \psi) * \phi = \int_M \psi * (-i\hbar)^n \sum_{k=0}^n b_{i_1 \dots i_k} \delta_{i_1} \dots \delta_{i_k} \phi \quad (A2.23)$$

Consider therefore the integral

$$\int_M \psi * (-i\hbar)^n \sum_{k=0}^n b_{i_1 \dots i_k} \phi_{|i_k \dots i_1} = \int_M \psi * (-i\hbar)^n \sum_{k=0}^n b_{i_1 \dots i_k} \phi_{|i_1 \dots i_k}, \quad (A2.24)$$

which upon applying lemma 2.3 yields

$$\int_M (-i\hbar)^n \sum_{k=0}^n (b_{i_1 \dots i_k} \psi^*)_{|i_1 \dots i_k} \phi, \quad (A2.25)$$

and upon applying lemma 2.4 becomes

$$\begin{aligned} & \int_M (-i\hbar)^n \sum_{k=0}^n \sum_{\ell=0}^k b_{i_{\ell+1} \dots i_k}^{i_1 \dots i_\ell} \psi^*_{|i_1 \dots i_\ell} \phi (-1)^k \\ &= \int_M ((-i\hbar)^n \sum_{\ell=0}^n \sum_{k=\ell}^n (-1)^{n+k} b_{i_{\ell+1} \dots i_k}^{i_1 \dots i_\ell} \delta_{i_1} \dots \delta_{i_\ell} \psi) * \phi. \end{aligned} \quad (A2.26)$$

Comparison of (A2.26) and (A2.23) yields the desired result.

Theorem 2.6: On the degree of indeterminacy in the general expression for $Q_0(A)$.

The recurrence relation

$$b_{i_1 \dots i_\ell}^{i_1 \dots i_\ell} = \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} b_{i_{\ell+1} \dots i_k}^{i_1 \dots i_k}, \quad \ell \in [0, n] \in \mathbb{N}, \quad (A2.27)$$

defines a unique set of tensors $b_{i_1 \dots i_\ell}^{i_1 \dots i_\ell}$, $\ell \in [0, n]$, if and only if the tensors

$$b_{i_1 \dots i_{n-2k}}^{i_1 \dots i_{n-2k}}, \quad k \in [0, [n/2]], \quad (A2.28)$$

are specified, these last being undetermined by the recurrence.

Proof: Rewriting (A2.27) as

$$b_{i_1 \dots i_\ell}^{i_1 \dots i_\ell} = (-1)^{n+\ell} b_{i_1 \dots i_\ell}^{i_1 \dots i_\ell} + \sum_{k=\ell+1}^n (-1)^{n+k} \binom{k}{\ell} b_{i_{\ell+1} \dots i_k}^{i_1 \dots i_k}, \quad (A2.29)$$

we perceive that the coefficients $b_{i_1 \dots i_\ell}^{i_1 \dots i_\ell}$ are undetermined by the coefficients $b_{i_1 \dots i_k}^{i_1 \dots i_k}$, $k > \ell$ if and only if $(-1)^{n+\ell} = 1$ or equivalently $\ell = n - 2k$, $k \in [0, [n/2]]$, the recurrence then reducing, as may be confirmed explicitly, to an identity. If these coefficients are given then the remaining coefficients are uniquely specified.

Theorem 2.7: On the symmetry of the auxiliary operators $\Xi_0(A)$.

The operator $\Xi_0(A)$ defined on the set $C_0^\infty(M)$ by the prescription

$$\Xi_0(A) = (-i\hbar)^n \sum_{k=0}^n \alpha_k^n a_{i_{k+1} \dots i_n}^{i_1 \dots i_n} \delta_{i_1} \dots \delta_{i_k}, \quad (A2.30)$$

in which the real-valued numerical coefficients α_k^n satisfy the recurrence relation

$$\alpha_\ell^n = \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} \alpha_k^n, \quad (A2.31)$$

together with the auxiliary condition $\alpha_n^n = 1$, is a symmetric operator.

Proof: We have by Theorem 2.5 that any symmetric operator needs only obey the recurrence (A2.27) whence by direct substitution of (A2.31) we deduce the required result. Explicitly, setting

$$b_{i_1 \dots i_k} = \alpha_k^n a_{i_1 \dots i_n | i_{k+1} \dots i_n}, \quad (\text{A2.32})$$

we have the equalities

$$\begin{aligned} \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} b_{i_1 \dots i_k | i_{\ell+1} \dots i_n} &= \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} (\alpha_k^n a_{i_1 \dots i_n | i_{k+1} \dots i_n})_{i_{\ell+1} \dots i_n} \\ &= \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} \alpha_k^n a_{i_1 \dots i_n | i_{\ell+1} \dots i_n} = b_{i_1 \dots i_\ell}. \end{aligned} \quad (\text{A2.33})$$

Theorem 2.8: On the canonical decomposition of $Q_o(A)$.

The most general symmetric operator $Q_o(A)$ has the canonical decomposition

$$Q_o(A) = \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} \Xi_o(B_{n-2k}), \quad (\text{A2.34})$$

in which the observable B_{n-2k} is the multilinear form

$$B_{n-2k} = b_{i_1 \dots i_{n-2k}} p_{i_1} \dots p_{i_{n-2k}}, \quad k \in [0, [n/2]]. \quad (\text{A2.35})$$

Moreover this decomposition may be related to the general tensorial representation of $Q_o(A)$ of (A2.20) in accordance with the equation

$$b_{i_1 \dots i_\ell} = \sum_{k=0}^{[n-\ell/2]} \alpha_\ell^{n-2k} b_{i_1 \dots i_{n-2k} | i_{\ell+1} \dots i_n}. \quad (\text{A2.36})$$

Proof: Consider firstly the expression (A2.34), which when combined with the definition of $\Xi_o(B_{n-2k})$ yields the double sum

$$Q_o(A) = \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} (-i\hbar)^{n-2k} \sum_{\ell=0}^{n-2k} \alpha_\ell^{n-2k} b_{i_1 \dots i_{n-2k} | i_{\ell+1} \dots i_n} \delta_{i_1} \dots \delta_{i_\ell}, \quad (\text{A2.37})$$

which upon rearranging becomes

$$(-i\hbar)^n \sum_{\ell=0}^n \left(\sum_{k=0}^{\lfloor \frac{n-\ell}{2} \rfloor} \alpha_{\ell}^{n-2k} b_{i_1 \dots i_{\ell+1} \dots i_{n-2k}}^{i_1 \dots i_{n-2k}} \right) \delta_{i_1} \dots \delta_{i_{\ell}}, \quad (\text{A2.38})$$

and from which the result (A2.36) follows.

It remains only to show that the quantities of (A2.36) obey the symmetry-induced recurrence relation (A2.27), the explicit calculation being as given below:

$$\begin{aligned} \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} b_{i_1 \dots i_{\ell+1} \dots i_k}^{i_1 \dots i_k} &= \sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} \sum_{j=0}^{\lfloor \frac{n-j}{2} \rfloor} \alpha_k^{n-2j} (b_{i_{k+1} \dots i_{n-2j}}^{i_1 \dots i_{n-2j}})_{i_{\ell+1} \dots} \\ &= \sum_{j=0}^{\lfloor \frac{n-\ell}{2} \rfloor} \left(\sum_{k=\ell}^n (-1)^{n+k} \binom{k}{\ell} \alpha_k^{n-2j} \right) b_{i_1 \dots i_{n-2j}}^{i_1 \dots i_{n-2j}} \\ &= \sum_{j=0}^{\lfloor \frac{n-\ell}{2} \rfloor} \alpha_{\ell}^{n-2j} b_{i_1 \dots i_{\ell+1} \dots i_{n-2j}}^{i_1 \dots i_{n-2j}} = b_{i_1 \dots i_{\ell}}^{i_1 \dots i_{\ell}}. \end{aligned} \quad (\text{A2.39})$$

Appendix 3: On Local Quantum Multilinear Momentum Observables.

We develop in this appendix all the proofs required in the third section of chapter 3.

Lemma 3.1: For all states $\psi \in C^\infty(\Gamma)$ and $\phi \in C^\infty_0(\Gamma)$ we have that

$$\int_{\Gamma} b^{i_1 \dots i_k} \phi_{|i_1 \dots i_k} \psi^* = (-1)^k \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)_{|i_1 \dots i_k} \phi. \quad (A3.1)$$

Proof: parallel to lemma 2.3 of the preceding appendix.

Lemma 3.2: The operator $\Xi^\infty_\Gamma(A)$ satisfies the inequality

$$\Xi^\infty_\Gamma(A) \subset (\Xi^0_\Gamma(A))^\dagger. \quad (A3.2)$$

Proof: It suffices to demonstrate that

$$\forall \phi \in D\Xi^0_\Gamma(A), \forall \psi \in D\Xi^\infty_\Gamma(A) \quad \langle \psi, \Xi^0_\Gamma(A)\phi \rangle = \langle \Xi^\infty_\Gamma(A)\psi, \phi \rangle. \quad (A3.3)$$

Explicitly we have that $\forall \phi \in D\Xi^0_\Gamma(A), \forall \psi \in DQ^\infty_\Gamma(A)$,

$$\langle \psi | \Xi^0_\Gamma(A)\phi \rangle = \int_M \psi^* \pi Q_0(A) \pi \phi = \int_{\Gamma} \psi^* Q_0(A) \pi \phi, \quad (A3.4)$$

and hence, noting that $\pi \phi \in C^\infty_0(\Gamma)$ and writing ϕ for $\pi \phi$, we deduce

$$\langle \psi | \Xi^0_\Gamma(A)\phi \rangle = \int_{\Gamma} \psi^* \sum_{k=0}^n (-i\hbar)^n \alpha_k^n a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \delta_{i_1} \dots \delta_{i_k} \phi. \quad (A3.5)$$

Further substituting from lemma 3.1 we obtain

$$\begin{aligned} \langle \psi | \Xi^0_\Gamma(A)\phi \rangle &= \sum_{k=0}^n \int_{\Gamma} (-i\hbar)^n \alpha_k^n (a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi^*)_{|i_1 \dots i_k} \phi (-1)^k \\ &= \sum_{k=0}^n \int_{\Gamma} (-i\hbar)^n \sum_{\ell=0}^k \alpha_k^n (a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n})_{|i_{\ell+1} \dots i_k} \psi^*_{|i_1 \dots i_\ell} \phi (-1)^k \binom{k}{\ell} \\ &= \sum_{\ell=0}^n \int_{\Gamma} [(-i\hbar)^n \left(\sum_{k=\ell}^n (-1)^{n+k} \alpha_k^n \binom{k}{\ell} \right) a_{|i_{\ell+1} \dots i_n}^{i_1 \dots i_n} \psi]^* \phi = \langle \Xi^\infty_\Gamma(A)\psi, \phi \rangle, \end{aligned} \quad (A3.6)$$

as required.

Theorem 3.3: The operator $Q_\Gamma^\infty(A)$ is contained in the adjoint of $Q_\Gamma^0(A)$, or symbolically

$$Q_\Gamma^\infty(A) = [Q_\Gamma^0(A)]^\dagger. \quad (\text{A3.7})$$

Proof: We have from the definition of $Q_\Gamma^0(A)$ that

$$[Q_\Gamma^0(A)]^\dagger \supset \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} (\Xi_\Gamma^0(B_{n-2k}))^\dagger, \quad (\text{A3.8})$$

and hence, from lemma 3.2 and the definition of $Q_\Gamma^\infty(A)$, that

$$[Q_\Gamma^0(A)]^\dagger \supset \sum_{k=0}^{[n/2]} (-i\hbar)^{2k} \Xi_\Gamma^\infty(B_{n-2k}) = Q_\Gamma^\infty(A). \quad (\text{A3.9})$$

Lemma 3.4: For all $\psi \in C^\infty(\Gamma)$, and for all fully symmetric $b^{i_1 \dots i_k}$, the following equalities hold in Γ :

$$(b^{i_1 \dots i_k} \psi)_{|i_1 \dots i_\ell} = \sum_{j=0}^{\ell} \binom{\ell}{j} b^{i_1 \dots i_k}_{|i_{j+1} \dots i_\ell} \psi_{|i_1 \dots i_j}. \quad (\text{A3.10})$$

Proof: by combinatorial methods analogous to these of lemma 2.4.

Lemma 3.5: For all $\phi, \psi \in C^\infty(\Gamma)$ the integral equations

$$\int_\Gamma b^{i_1 \dots i_k} \phi_{|i_1 \dots i_k} \psi^* = R(\ell, \partial\Gamma) + (-1)^\ell \int_\Gamma (b^{i_1 \dots i_k} \psi^*)_{|i_1 \dots i_\ell} \phi_{|i_{\ell+1} \dots i_k}, \quad (\text{A3.11})$$

in which $R(\ell, \partial\Gamma)$ is the surface integral

$$R(\ell, \partial\Gamma) = \int_{\partial\Gamma} \sum_{j=0}^{\ell-1} (-1)^j (b^{i_1 \dots i_k} \psi^*)_{|i_1 \dots i_j} \phi_{|i_{j+1} \dots i_{k-1}} \hat{n}_{i_k} d\sigma, \quad (\text{A3.12})$$

are satisfied for all ℓ : $1 \leq \ell \leq k$.

Proof: Note that $b^{i_1 \dots i_k}$ is fully symmetric, and proceed by induction on ℓ . The identity

$$\begin{aligned} \int_{\Gamma} b^{i_1 \dots i_k} \phi|_{i_1 \dots i_k} \psi^* &= \int_{\Gamma} (b^{i_1 \dots i_k} \phi|_{i_1 \dots i_{k-1}} \psi^*)|_{i_k} \quad (A3.13) \\ &- \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_k} \phi|_{i_1 \dots i_{k-1}}, \end{aligned}$$

yields, upon application of the divergence theorem^(a4), the result

$$\begin{aligned} \int_{\Gamma} b^{i_1 \dots i_k} \phi|_{i_1 \dots i_k} \psi^* &= \int_{\partial \Gamma} b^{i_1 \dots i_k} \phi|_{i_1 \dots i_{k-1}} \psi^* \hat{n}_{i_k} d\sigma \quad (A3.14) \\ &+ (-1) \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_k} \phi|_{i_1 \dots i_{k-1}} \end{aligned}$$

which is identically the expression (A3.11) with $\ell = 1$.

If, moreover, the identities (A3.11) are assumed to hold for $\ell \leq \rho-1$, with $\rho \leq k$, then we have that

$$\begin{aligned} \int_{\Gamma} b^{i_1 \dots i_k} \phi|_{i_1 \dots i_k} \psi^* &= R(\ell-1, \partial \Gamma) + (-1)^{\ell-1} \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho-1}} \phi|_{i_{\rho} \dots i_k} \quad (A3.15) \\ &= R(\ell-1, \partial \Gamma) + (-1)^{\ell-1} \int_{\Gamma} [(b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho-1}} \phi|_{i_{\rho} \dots i_{k-1}}]|_{i_k} \\ &\quad + (-1)^{\ell} \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho-1}} \phi|_{i_{\rho} \dots i_{k-1}} \\ &= R(\ell-1, \partial \Gamma) + (-1)^{\ell-1} \int_{\partial \Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho-1}} \phi|_{i_{\rho} \dots i_{k-1}} \hat{n}_{i_k} d\sigma \\ &\quad + (-1)^{\ell} \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho}} \phi|_{i_{\rho+1} \dots i_k} \\ &= R(\ell, \partial \Gamma) + (-1)^{\ell} \int_{\Gamma} (b^{i_1 \dots i_k} \psi^*)|_{i_1 \dots i_{\rho}} \phi|_{i_{\rho+1} \dots i_k}, \end{aligned}$$

which last is of the desired form (A3.11), so that the result has been demonstrated.

Theorem 3.6: On the symmetry-induced boundary-conditions of $\Xi_{\Gamma}^{\infty}(A)$.

The operator $\Xi_{\Gamma}^{\infty}(A)$ is symmetric if and only if for all states $\psi, \phi \in C^{\infty}(\Gamma)$ we have

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} \beta_{\rho k}^n \int_{\partial \Gamma} a_{|i_{\rho+k+2} \dots i_n}^{i_1 \dots i_n} \psi^*_{|i_1 \dots i_{\rho}} \phi_{|i_{\rho+1} \dots i_{\rho+k}} \hat{n}_{i_{\rho+k+1}} d\sigma = 0, \quad (A3.16)$$

in which the quantities $\beta_{\rho k}^n$ are determined by the relation

$$\beta_{\rho k}^n = \sum_{\ell=\rho+k+1}^n \alpha_{\ell}^n (-1)^{\ell-1-k} \binom{\ell-1-k}{\rho}. \quad (A3.17)$$

Proof: Substituting for $\Xi_{\Gamma}^{\infty}(A)$ from its definition, we deduce that,
 $\forall \psi, \phi \in C^{\infty}(\Gamma), \langle \psi | \Xi_{\Gamma}^{\infty}(A) \phi \rangle =$

$$(-i\hbar)^n \int_{\Gamma} \psi^* \sum_{k=0}^n \alpha_k^n a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \phi_{|i_1 \dots i_k}, \quad (A3.18)$$

which result yields in its turn, upon application of lemma 3.5 with $b_{|i_1 \dots i_k}^{i_1 \dots i_k} = a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n}$ and $\ell = k$, the equivalent expression

$$\begin{aligned} & (-i\hbar)^n \sum_{k=0}^n \alpha_k^n \left[\sum_{j=0}^{k-1} (-1)^j \int_{\partial \Gamma} (a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi^*)_{|i_1 \dots i_j} \phi_{|i_{j+1} \dots i_{k-1}} \hat{n}_{i_k} d\sigma \right. \\ & \quad \left. + (-1)^k \int_{\Gamma} (a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi^*)_{|i_1 \dots i_k} \phi \right]. \end{aligned} \quad (A3.19)$$

Apply lemma 3.4 to the terms of (A3.19) and infer that

$$\langle \psi | \Xi_{\Gamma}^{\infty}(A) \phi \rangle = (-i\hbar)^n \quad (A3.20)$$

$$\begin{aligned} & \sum_{k=0}^n \sum_{j=0}^{k-1} (-1)^j \int_{\partial \Gamma} \alpha_k^n \sum_{\rho=0}^j \binom{j}{\rho} a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} |i_{\rho+1} \dots i_j \psi^*_{|i_1 \dots i_{\rho}} \phi_{|i_{j+1} \dots i_{k-1}} \hat{n}_{i_k} \\ & + (-i\hbar)^n \sum_{k=0}^n \sum_{\rho=0}^k \alpha_k^n (-1)^k \int_{\Gamma} a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} |i_{\rho+1} \dots i_k \psi^*_{|i_1 \dots i_{\rho}} \phi_{\rho}^{(k)}. \end{aligned}$$

Hence by interchange of the order of summation deduce that the second (volume) integral becomes

$$\begin{aligned}
& (-i\hbar)^n \sum_{\rho=0}^n \left[\sum_{k=\rho}^n \alpha_k^n (-1)^k \binom{k}{\rho} \right] \int_{\Gamma} a_{|i_{\rho+1} \dots i_n}^{i_1 \dots i_n} \psi_{|i_1 \dots i_{\rho}}^* \phi \quad (A3.21) \\
& = \int_{\Gamma} [(-i\hbar)^n \sum_{\rho=0}^n \alpha_{\rho}^n a_{|i_1 \dots i_n}^{i_1 \dots i_n} \psi_{|i_1 \dots i_{\rho}}^*] \phi = \langle \Xi_{\Gamma}^{\infty}(A) \psi, \phi \rangle,
\end{aligned}$$

so that we perceive that the symmetry condition is the vanishing of the surface integral of equation (A3.20). Explicitly this is

$$\sum_{k=0}^n \sum_{j=0}^{k-1} \sum_{\rho=0}^j \int_{\partial \Gamma} (-1)^j \alpha_k^n \binom{j}{\rho} a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi_{|i_{\rho+1} \dots i_j}^* \phi_{|i_1 \dots i_{\rho}} \hat{n}_{i_{j+1} \dots i_{k-1} i_k} d\sigma = 0$$

Introduce the index variable $\ell = k-1-j$ so that the above expression becomes

$$\sum_{k=0}^n \sum_{\ell=0}^{k-1} \sum_{\rho=0}^{k-\ell-1} \int_{\partial \Gamma} (-1)^{k-\ell-1} \alpha_k^n \binom{k-\ell-1}{\rho} a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi_{|i_{\rho+1} \dots i_{k-\ell-1}}^* \phi_{|i_1 \dots i_{\rho}} \hat{n}_{i_{k-\ell} \dots i_{k-1} i_k} d\sigma.$$

Interchange the order of summation (twice) to obtain

$$\sum_{\ell=0}^{n-1} \sum_{\rho=0}^{n-1-\ell} \sum_{k=\ell+\rho+1}^n \int_{\partial \Gamma} [(-1)^{k-\ell-1} \alpha_k^n \binom{k-\ell-1}{\rho}] a_{|i_{k+1} \dots i_n}^{i_1 \dots i_n} \psi_{|i_{\rho+1} \dots i_{k-\ell-1}}^* \phi_{|i_1 \dots i_{\rho}} \hat{n}_{i_{k-\ell} \dots i_{k-1} i_k} d\sigma$$

and, noting that since $a_{|i_1 \dots i_n}^{i_1 \dots i_n}$ is fully symmetric one may arbitrarily rearrange the covariant differentiations, deduce

$$\sum_{\ell=0}^{n-1} \sum_{\rho=0}^{n-1-\ell} \sum_{k=\ell+\rho+1}^n \int_{\partial \Gamma} [(-1)^{k-\ell-1} \alpha_k^n \binom{k-\ell-1}{\rho}] a_{|i_{\ell+\rho+2} \dots i_n}^{i_1 \dots i_n} \psi_{|i_1 \dots i_{\rho}}^* \phi_{|i_{\rho+1} \dots i_{\ell+\rho}} \hat{n}_{i_{\ell+\rho+1}} d\sigma$$

as the symmetry integral. Finally substituting from the definition of $\beta_{\rho\ell}^n$ we obtain as required the final representation

$$\sum_{\ell=0}^{n-1} \sum_{\rho=0}^{n-1-\ell} \beta_{\rho\ell}^n \int_{\partial \Gamma} a_{|i_{\ell+\rho+2} \dots i_n}^{i_1 \dots i_n} \psi_{|i_1 \dots i_{\rho}}^* \phi_{|i_{\rho+1} \dots i_{\ell+\rho}} \hat{n}_{i_{\ell+\rho+1}} d\sigma = 0. \quad (A3.22)$$

Theorem 3.7: On the symmetry induced boundary conditions of $Q_\Gamma^\infty(A)$.

The operator $Q_\Gamma^\infty(A)$ is symmetric if and only if, for all $\psi, \phi \in C^\infty(\Gamma)$, we have

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} \int_{\partial\Gamma} y_{n\rho k}^{i_1 \dots i_{\rho+k+1}} \psi_{|i_1 \dots i_\rho}^* \phi_{|i_{\rho+1} \dots i_{\rho+k}} \hat{n}_{i_{\rho+k+1}} d\sigma = 0, \quad (A3.23)$$

in which

$$y_{n\rho k}^{i_1 \dots i_{\rho+k+1}} = \sum_{i=0}^{\lfloor \frac{n-1-k-\rho}{2} \rfloor} \beta_{\rho k}^{n-2i} b_{|i_{\rho+k+2} \dots i_{n-2i}}^{i_1 \dots i_{n-2i}}. \quad (A3.24)$$

Proof: We have that by definition

$$Q_\Gamma^\infty(A) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-i\hbar)^{2k} \equiv_\Gamma^\infty (B_{n-2k}), \quad (A3.25)$$

and hence, parallel to the analysis of the previous theorem

3.6, we deduce that $Q_\Gamma^\infty(A)$ is symmetric if and only if

$$\sum_{k=0}^{\lfloor n/2 \rfloor} \sum_{\ell=0}^{n-2k-1} \sum_{\rho=0}^{n-2k-1-\ell} \beta_{\rho\ell}^{n-2k} \int_{\partial\Gamma} b_{|i_{\ell+\rho+2} \dots i_{n-2k}}^{i_1 \dots i_{n-2k}} \psi_{|i_1 \dots i_\rho}^* \phi_{|i_{\rho+1} \dots i_{\rho+\ell}} \hat{n}_{i_{\rho+\ell+1}} d\sigma = 0. \quad (A3.26)$$

This may be rewritten by two interchanges of the order of summation as

$$\sum_{\ell=0}^{n-1} \sum_{\rho=0}^{n-1-\ell} \int_{\partial\Gamma} \sum_{k=0}^{\lfloor \frac{n-1-\rho-\ell}{2} \rfloor} \beta_{\rho\ell}^{n-2k} b_{|i_{\ell+\rho+2} \dots i_{n-2k}}^{i_1 \dots i_{n-2k}} \psi_{|i_1 \dots i_\rho}^* \phi_{|i_{\rho+1} \dots i_{\rho+\ell}} \hat{n}_{i_{\rho+\ell+1}} d\sigma = 0, \quad (A3.27)$$

which upon substitution for the innermost sum yields the required result.

Theorem 3.8: On the canonical decomposition of the prescribed operators $\equiv_o(A)$.

The operators $\equiv_o(A)$ defined in terms of the differential expressions

$$\Xi_0(A) = \begin{cases} (-i\hbar)^{n=2\ell} \delta_{i_1} \dots \delta_{i_\ell} a^{i_1 \dots i_{2\ell}} \delta_{i_{\ell+1}} \dots \delta_{i_{2\ell}} & , \ell \in [1, \infty], \\ (-i\hbar)^{n=2\ell+1} \delta_{i_1} \dots \delta_{i_\ell} \frac{1}{2} \{ a^{i_1 \dots i_{2\ell+1}} \delta_{i_{\ell+1}} \} \delta_{i_{\ell+2}} \dots \delta_{i_{2\ell+1}} & , \ell \in [0, \infty], \end{cases} \quad (A3.28)$$

when expressed in the canonical form

$$\Xi_0(A) = (-i\hbar)^n \sum_{k=0}^n \alpha_k^n a^{i_1 \dots i_n} \delta_{i_{k+1}} \dots \delta_{i_n} \delta_{i_1} \dots \delta_{i_k}, \quad (A3.29)$$

yield the following values for the coefficients α_k^n :

$$\alpha_k^{n=2\ell} = \binom{\ell}{k-\ell}, \quad \alpha_k^{n=2\ell+1} = \binom{\ell+1}{k-\ell} - \frac{1}{2} \binom{\ell}{k-\ell}. \quad (A3.30)$$

Proof: For the case of n even we have that by definition, and for all $\psi \in C_0^\infty(M)$,

$$\Xi_0(A)\psi = (-i\hbar)^{n=2\ell} (a^{i_1 \dots i_{2\ell}} \psi_{|i_1 \dots i_\ell} |_{i_{\ell+1} \dots i_{2\ell}}), \quad (A3.31)$$

which expression may be reduced, by noting the full symmetry of $a^{i_1 \dots i_{2\ell}}$, to

$$\Xi_0(A)\psi = (-i\hbar)^{2\ell} \sum_{k=0}^{\ell} \binom{\ell}{k} a^{i_1 \dots i_{2\ell}} \psi_{|i_{k+1} \dots i_\ell} |_{i_1 \dots i_k} |_{i_{\ell+1} \dots i_{2\ell}}, \quad (A3.32)$$

or equivalently, by noting our convention regarding "out of range" binomial coefficients, to

$$\Xi_0(A)\psi = (-i\hbar)^{2\ell} \sum_{k=0}^{2\ell} \binom{\ell}{k-\ell} a^{i_1 \dots i_{2\ell}} \psi_{|i_{k+1} \dots i_{2\ell}} |_{i_1 \dots i_k}, \quad (A3.33)$$

from which last the result $\alpha_k^{2\ell} = \binom{\ell}{k-\ell}$ is immediate.

For the case of n odd we have, for all $\psi \in C_0^\infty(M)$, that

$$\begin{aligned} \Xi_0(A)\psi &= (-i\hbar)^{n=2\ell+1} \frac{1}{2} [2(a^{i_1 \dots i_{2\ell+1}} \psi | i_1 \dots i_{\ell+1}) | i_{\ell+2} \dots i_{2\ell+1} \\ &\quad + (a^{i_1 \dots i_{2\ell+1}} \psi | i_1 \dots i_{\ell}) | i_{\ell+1} \dots i_{2\ell+1}] , \end{aligned} \quad (A3.34)$$

which is readily shown to have the expansion

$$\begin{aligned} \Xi_0(A)\psi &= (-i\hbar)^{2\ell+1} \frac{1}{2} [2 \sum_{k=0}^{\ell} \binom{\ell}{k} a^{i_1 \dots i_{2\ell+1}} \psi | i_{\ell+k+2} \dots i_{2\ell+1} | i_1 \dots i_k | i_{k+1} \dots i_{\ell+k+1} \\ &\quad + \sum_{k=0}^{\ell+1} \binom{\ell+1}{k} a^{i_1 \dots i_{2\ell+1}} \psi | i_{\ell+k+1} \dots i_{2\ell+1} | i_1 \dots i_k | i_{k+1} \dots i_{\ell+k}]] , \end{aligned} \quad (A3.35)$$

This last, after a brief calculation, yields

$$\begin{aligned} \Xi_0(A)\psi &= (-i\hbar)^{2\ell+1} \frac{1}{2} [2 \sum_{k=\ell+1}^{2\ell+1} \binom{\ell}{k-\ell-1} a^{i_1 \dots i_{2\ell+1}} \psi | i_{k+1} \dots i_{2\ell+1} | i_1 \dots i_k \\ &\quad + \sum_{k=\ell}^{2\ell+1} \binom{\ell}{k-\ell} a^{i_1 \dots i_{2\ell+1}} \psi | i_{k+1} \dots i_{2\ell+1} | i_1 \dots i_k]] , \end{aligned} \quad (A3.36)$$

so that immediately

$$\alpha_k^{2\ell+1} = 2 \binom{\ell}{k-\ell-1} + \frac{1}{2} \binom{\ell}{k-\ell} = \binom{\ell+1}{k-\ell} - \frac{1}{2} \binom{\ell}{k-\ell} , \quad (A3.37)$$

as required.

note: The coefficients $\alpha_k^{2\ell+1}$ are most readily generated by a construction analogous to Pascal's triangle and based upon the recurrence

$$\alpha_k^{2\ell+1} = \alpha_{k-1}^{2\ell-1} + \alpha_{k-2}^{2\ell-1} , \quad (A3.38)$$

and the initial conditions

$$\alpha_1^1 = 1 , \quad \alpha_0^1 = \frac{1}{2} . \quad (A3.39)$$

Lemma 3.9: The coefficients α_k^n of (A3.30) can be written as the following contour integrals:

$$\alpha_k^{2\ell} = \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m x^{-(k+1)} dx, \quad (\text{A3.40})$$

$$\alpha_k^{2\ell+1} = \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m (\frac{1}{2}+x) x^{-(k+1)} dx.$$

Proof: For the case of even n we have that

$$x^m (1+x)^m = \sum_{\ell=m}^{2m} \binom{m}{\ell-m} x^\ell, \quad (\text{A3.41})$$

is a generating function for the coefficients $\binom{m}{\ell-m}$, and hence it is immediate from the residue theorem^(a5) that

$$\alpha_k^{2m} = \binom{m}{k-m} = \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m x^{-(1+k)} dx. \quad (\text{A3.42})$$

For the case of n odd we have that

$$x^m (1+x)^m (\frac{1}{2}+x) = \sum_{\ell=m}^{2m+1} \left[\binom{m+1}{\ell-m} - \frac{1}{2} \binom{m}{\ell-m} \right] x^\ell, \quad (\text{A3.43})$$

is a generating function for the coefficients $\alpha_k^{2\ell+1}$ from which the result follows directly from the residue theorem.

Theorem 3.10: On the symmetry of the prescribed operators $\equiv_o(A)$.

The operators $\equiv_o(A)$ of (A3.28) are symmetric.

Proof: We shall demonstrate equivalently that the coefficients α_k^n above obey the symmetry induced recurrence (A2.31).

For n even we have that, by lemma 3.9,

$$\begin{aligned} \sum_{k=\ell}^{2m} (-1)^k \binom{k}{\ell} \binom{m}{k-m} &= \sum_{k=\ell}^{2m} (-1)^k \binom{k}{\ell} \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m x^{-(1+k)} dx \\ &= \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m \sum_{k=\ell}^{\infty} (-1)^k \binom{k}{\ell} x^{-(1+k)} dx, \end{aligned} \quad (\text{A3.44})$$

where the addition terms in the sum, $k \in [2m+1, \infty]$, do not

contribute to the residue. Further we have the identity^(a6)

$$(-1)^\ell (1+x)^{-(1+\ell)} = \sum_{k=\ell}^{\infty} (-1)^k \binom{k}{\ell} x^{-(1+k)}, \quad |x| > 1, \quad (\text{A3.45})$$

and hence we may deduce that

$$\begin{aligned} \sum_{k=\ell}^{2m} (-1)^k \binom{k}{\ell} \binom{m}{k-m} &= \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m (-1)^\ell (1+x)^{-(1+\ell)} dx \\ &= \frac{1}{2\pi i} \oint_{x=0} x^m (-1)^\ell \sum_{k=\ell-m}^{\infty} (-1)^k \binom{k}{\ell-m} (-1)^{\ell-m-k} x^{-(1+k)} dx = \binom{m}{\ell-m}, \end{aligned} \quad (\text{A3.46})$$

which is the desired result.

For n odd we have similarly that, by lemma 3.9,

$$\begin{aligned} \sum_{k=\ell}^{2m+1} \alpha_k^{2m+1} (-1)^k \binom{k}{\ell} &= \sum_{k=\ell}^{2m+1} (-1)^k \binom{k}{\ell} \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m \left(\frac{1}{2}+x\right) x^{-(1+k)} dx \\ &= \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m \left(\frac{1}{2}+x\right) \sum_{k=\ell}^{\infty} (-1)^k \binom{k}{\ell} x^{-(1+k)}, \end{aligned} \quad (\text{A3.47})$$

the additional terms augmenting the summation not affecting the residue.

Thus by the identity (A3.45) we may infer that

$$\begin{aligned} \sum_{k=\ell}^{2m+1} \alpha_k^{2m+1} (-1)^k \binom{k}{\ell} &= \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m \left(\frac{1}{2}+x\right) (-1)^\ell (1+x)^{-(1+\ell)} dx \\ &= \frac{1}{2\pi i} \oint_{x=0} x^m \left(\frac{1}{2}+x\right) (-1)^\ell \sum_{k=\ell-m}^{\infty} (-1)^k \binom{k}{\ell-m} (-1)^{\ell-m-k} x^{-(1+k)} dx \\ &= (-1)^{2m+1} \left[\binom{m+1}{\ell-m} - \frac{1}{2} \binom{m}{\ell-m} \right] = (-1)^n \alpha_\ell^{2m+1}, \end{aligned} \quad (\text{A3.48})$$

as required.

Theorem 3.11: On the explicit forms of the coefficients $\beta_{\rho k}^n$ generated by the above α_k^n .

The coefficients $\beta_{\rho k}^n$ determined by the quantities α_k^n in accordance with the equation

$$\beta_{\rho k}^n = \sum_{\ell=\rho+k+1}^n \alpha_\ell^n (-1)^{\ell-1-k} \binom{\ell-1-k}{\rho}, \quad (\text{A3.49})$$

are given explicitly by the prescriptions

$$\beta_{\rho k}^{n=2m} = \begin{cases} (-1)^\rho \binom{m-\rho-1}{k-m}, & \rho < m, m \leq k, \\ -(-1)^k \binom{m-k-1}{\rho-m}, & k < m, m \leq \rho, \end{cases} \quad (\text{A3.50})$$

and

$$\beta_{\rho k}^{n=2m+1} = \begin{cases} (-1)^\rho \left[\binom{m-\rho}{k-m} - \frac{1}{2} \binom{m-\rho-1}{k-m} \right], & \rho < m, m \leq k, \\ (-1)^k \left[\binom{m-k}{\rho-m} - \frac{1}{2} \binom{m-k-1}{\rho-m} \right], & k < m, m \leq \rho, \end{cases} \quad (\text{A3.51})$$

all the other coefficients being zero.

Proof: We employ contour integration and the residue theorem and shall require the identity

$$x^\rho (1+x)^{-(\rho+1)} = \sum_{\sigma=0}^{\infty} (-1)^\sigma \binom{\sigma+\rho}{\rho} x^{-(1+\sigma)}, \quad |x| > 1, \quad (\text{A3.52})$$

which we state without proof.

For the case of n even we have by definition and by application of lemma 3.9 that

$$\beta_{\rho k}^{2m} = \sum_{\ell=\rho+k+1}^{2m} (-1)^{\ell-1-k} \binom{\ell-1-k}{\rho} \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m x^{-(1+\ell)} dx. \quad (\text{A3.53})$$

Thus, letting $\sigma = \ell - (\rho+k+1)$ and $\ell = \sigma + \rho + k + 1$, and extending the upper limit of summation to infinity, we deduce

$$\beta_{\rho k}^{2m} = \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^m (-1)^\rho x^{-(1+\rho+k)} \sum_{\sigma=0}^{\infty} (-1)^\sigma \binom{\sigma+\rho}{\rho} x^{-(1+\sigma)} dx. \quad (\text{A3.54})$$

Hence, noting the identity (A3.52), we obtain the contour integral representation

$$\beta_{\rho k}^{2m} = \frac{(-1)^\rho}{2\pi i} \oint_{x=0} \frac{x^m (1+x)^m}{x^{k+1} (1+x)^{\rho+1}} dx, \quad (A3.55)$$

from which the result (A3.50) follows by means of careful application of the residue theorem.

Similarly for n odd we obtain parallel to (A3.53) that

$$\beta_{\rho k}^{2m+1} = \frac{1}{2\pi i} \oint_{x=0} x^m (1+x)^{m(\frac{1}{2}+x)} (-1)^\rho x^{-(1+k+\rho)} \sum_{\sigma=0}^{\infty} (-1)^\sigma \binom{\sigma+\rho}{\rho} x^{-(1+\sigma)} dx, \quad (A3.56)$$

and substituting from (A3.52) that

$$\beta_{\rho k}^{2m+1} = \frac{(-1)^\rho}{2\pi i} \oint_{x=0} \frac{x^m (1+x)^{m(\frac{1}{2}+x)}}{x^{k+1} (1+x)^{\rho+1}} dx, \quad (A3.57)$$

the final part of the proof following from the residue theorem.

Theorem 3.12: Sufficient conditions for the quantizability of the local observables $Q_\Gamma^0(A)$.

The boundary conditions

$$n_{i_{\rho+k+1}} y_{n\rho k}^{i_1 \dots i_{\rho+k+1}} (\partial \Gamma) = \sum_{i=0}^{\lfloor \frac{n-1-\rho-k}{2} \rfloor} n_{i_{\rho+k+1}} \beta_{\rho k}^{n-2i} b_{i_{\rho+k+2} \dots i_{n-2i}}^{i_1 \dots i_{n-2i}} (\partial \Gamma) = 0, \quad (A3.57)$$

are equivalent to the boundary conditions

$$n_{i_{\rho+1}} b_{i_1 \dots i_{\rho}}^{i_1 \dots i_{n-2\sigma}} (\partial \Gamma) = 0, \quad 0 \leq \rho \leq \lfloor n/2 - \frac{1}{4} \rfloor - \sigma, \quad 0 \leq \sigma \leq \lfloor n/2 - \frac{1}{4} \rfloor. \quad (A3.58)$$

Proof: For the case of n even, let $n = 2m$, $\rho + k + 1 = 2m - \ell$, $\ell \in [0, m-1]$, and assuming without loss of generality that $\rho < k$ let

$$\rho = m - 1 - \ell, \quad k = m. \quad (A3.59)$$

Then from A3.50 we have that

$$\beta_{\rho k}^{2(m-i)} = (-1)^\rho \binom{\ell-i}{\ell+i} = \begin{cases} 1, & i = 0 \\ 0, & i \neq 0 \end{cases}, \quad (A3.60)$$

which upon substitution into (A3.57) yields that

$$(-1)^{2m-\ell} n_{i_{2m-\ell}} b_{i_{2m-\ell} | i_1 \dots i_{2m}}^{i_1 \dots i_{2m}} (\partial \Gamma) = 0, \ell \in [0, m-1], \quad (\text{A3.61})$$

or upon rearrangement

$$n_{i_{\rho+1}} b_{i_{\rho+1} | i_1 \dots i_{\rho}}^{i_1 \dots i_{2m}} (\partial \Gamma) = 0, \rho \in [0, [n/2]-1]. \quad (\text{A3.62})$$

Moreover it follows immediately from (A3.50) with $\rho < k$ that

$\beta_{\rho+k+1}^{2m} = 0$, $\rho+k+1 \leq m$ and hence, applying (A3.61), the sum (A3.57) becomes

$$\sum_{i=1}^{\lfloor \frac{n-1-\rho-k}{2} \rfloor} n_{i_{\rho+k+1}} \beta_{\rho k}^{n-2i} b_{i_{\rho+k+2} \dots i_{n-2i}}^{i_1 \dots i_{n-2i}} (\partial \Gamma) = 0. \quad (\text{A3.63})$$

Finally, setting $i \rightarrow i-1$, obtain the reduced sum

$$\sum_{i=0}^{\lfloor \frac{2(m-1)-1-\rho-k}{2} \rfloor} n_{i_{\rho+k+1}} \beta_{\rho k}^{2(m-1)-2i} b_{i_{\rho+k+2} \dots i_{2(m-1)-2i}}^{i_1 \dots i_{2(m-1)-2i}} (\partial \Gamma) = 0, \quad (\text{A3.64})$$

from which the result follows by induction.

The proof is similar for n odd.

Theorem 3.13: Necessary and sufficient conditions for the essential self-adjointness of $Q_{\Gamma}^0(A)$ on a one-dimensional manifold.

The boundary conditions

$$b_{i_1 \dots i_{\rho}}^{i_1 \dots i_{n-2\sigma}}(a) = b_{i_1 \dots i_{\rho}}^{i_1 \dots i_{n-2\sigma}}(b) = 0, \quad (\text{A3.65})$$

$$0 \leq \rho \leq [n/2-1]-\sigma, 0 \leq \sigma \leq [n/2-1],$$

are both necessary and sufficient that $Q_{\Gamma}^0(A)$ is essentially self-adjoint in the finite subset (a,b) of a one-dimensional manifold (M,G) .

Proof: Sufficiency is immediate from theorem 3.12. To prove necessity we proceed as follows:

The symmetry boundary conditions of the operator $Q_\Gamma^0(A)$ are given for the case of a one-dimensional manifold by the specialization of (A3.23),

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} y_{npk} \Delta^\rho \psi^* \Delta^k \phi \Big|_a^b = 0, \quad \forall \psi, \phi \in C^\infty(\Gamma) \quad (A3.66)$$

in which the operator Δ is that of covariant differentiation.

Suppose now that the wave-functions $\psi(x) \in C^\infty[a, b]$ obey the boundary conditions

$$\Delta^k \phi(b) = \sum_{\ell=0}^{n-1} \omega_\ell^k \Delta^\ell \phi(a), \quad k \in [0, n-1], \quad \omega_\ell^k \in \mathbb{C}, \quad (A3.67)$$

then by substituting into (A3.66) we deduce that the symmetry condition is obeyed if and only if

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} \sum_{\ell=0}^{n-1} (y_{npk}(b) \Delta^\rho \psi^*(b) \omega_\ell^k - y_{npk}(a) \Delta^\rho \psi^*(a) \delta_\ell^k) \Delta^\ell \phi(a) = 0, \quad (A3.68)$$

hence, since the quantities $\Delta^\ell \phi(a)$ are arbitrary, we obtain the adjoint boundary conditions,

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} (y_{npk}^n(b) \Delta^\rho \psi^*(b) \omega_\ell^k - y_{npk}(a) \Delta^\rho \psi^*(a) \delta_\ell^k) = 0. \quad (A3.69)$$

We require that the boundary conditions (A3.69) should determine a self-adjoint extension of $Q_\Gamma^0(A)$, so that the quantities $\Delta^k \psi(b)$ must obey the same boundary conditions as $\Delta^k \phi(b)$ namely (A3.67). Thus by substitution we deduce that

$$\sum_{k=0}^{n-1} \sum_{\rho=0}^{n-1-k} (y_{npk}(b) \omega_\ell^k \omega_m^{*\rho} - y_{npk}(a) \delta_\ell^k \delta_m^\rho) = 0. \quad (A3.70)$$

If, therefore, there exist any non-trivial solutions $\omega_\ell^k \neq 0$, then an infinite family of solutions is given by the coefficients

$\eta_{\ell}^k = e^{i\beta \omega_{\ell}^k}$, so that there can exist a unique self-adjoint extension of $Q_{\Gamma}^0(A)$ only if $\omega_{\ell}^k = 0$, which implies directly that

$$y_{n\ell m}(a) = 0. \quad (\text{A3.71})$$

A parallel analysis shows also that $y_{n\ell m}(b) = 0$, and hence from theorem 3.12 we infer the desired result.

Appendix 4: On the Determination of the Tensor Quantities $B_{n-2k}^{(A)}$,
 $k \in [0, [n/2]]$.

We develop in this section all the proofs required for the fourth section of chapter 3.

Theorem 4.1: On the determination for the bilinear constants of motion of the quantity $c(a^{ij})$.

The requirement that the quantization rule

$$[Q(g^{ij}_{p_i p_j}), Q(a^{ij}_{p_i p_j})] = 0, \quad (A4.1)$$

be satisfied for constants, $a^{ij}_{p_i p_j}$, of the free classical motion results in the explicit expression for $Q(a^{ij}_{p_i p_j})$,

$$Q(a^{ij}_{p_i p_j}) = (-i\hbar)^2 (a^{ij}_{\delta_i \delta_j} + a^{ij}_{|j \delta_i} + \frac{1}{2} a^{ij}_{|i |j}) . \quad (A4.2)$$

Proof: We prove this result in full only for a Euclidean space, the general proof being sketched. We have that the general form of any bilinear quantum observable is simply

$$Q(a^{ij}_{p_i p_j}) = (-i\hbar)^2 (a^{ij}_{\delta_i \delta_j} + a^{ij}_{|j \delta_i} + c(a^{ij})) ; \quad (A4.3)$$

whence by substitution in (A4.1) we obtain the quantization prescription

$$\begin{aligned} \forall \psi \in C^\infty_0(M); \quad & g^{ij} a^{k\ell} (\psi_{|k\ell ij} - \psi_{|ij k\ell}) \\ & + 2g^{ij} a^{k\ell}_{|j} \psi_{|k\ell i} + g^{ij} a^{k\ell} (\psi_{|kij} - \psi_{|ijk}) \\ & + g^{ij} a^{k\ell}_{|ij} \psi_{|k\ell} + 2g^{ij} a^{k\ell}_{|lj} \psi_{|ki} \\ & + g^{ij} a^{k\ell}_{|lij} \psi_{|k} + 2g^{ij} c_{|j} \psi_{|i} + g^{ij} c_{|ij} \psi = 0 \end{aligned} \quad (A4.4)$$

which determines the function $c(a^{ij})$.

We have in addition and by hypothesis the requirement that $a^{ij}_{p_i p_j}$ is a constant of the free classical motion, that is that

$$\{g^{ij}p_i p_j, a^{ij}_{|p_i p_j}\} = -2 a^{k\ell}_{|\mu} g^{\mu j} p_j p_k p_\ell, \quad (\text{A4.5})$$

which yields upon symmetrization the equivalent constraint

$$g^{\mu j} a^{k\ell}_{|\mu} + g^{\ell\mu} a^{jk}_{|\mu} + g^{k\mu} a^{\ell j}_{|\mu} = 0. \quad (\text{A4.6})$$

In the special case of a Euclidean space covariant differentiation is identical to partial differentiation, and hence substituting (A4.6) into (A4.4), and cancelling the vanishing terms we obtain the residue

$$(-i\hbar)^3 [(g^{ij} a^{\mu\ell}_{|\ell ij} + 2c^{\mu})\psi_{,\mu} + \frac{1}{2}(g^{ij} a^{\mu\ell}_{|\ell ij} + 2c^{\mu})_{,\mu}] \psi = 0. \quad (\text{A4.7})$$

It is now immediate that

$$g^{ij} a^{\mu\ell}_{|\ell ij} + 2c^{\mu} = 0, \quad (\text{A4.8})$$

or equivalently that

$$(c - \frac{1}{4} a^{i,j}_{i,j})_{,\mu} = 0 \quad (\text{A4.9})$$

and hence the result (A4.2) follows.

In the general case the residue analogous to (A4.7) can be obtained by employing Ricci's identities^(a7)

$$a_{i_1 \dots i_m | jk} - a_{i_1 \dots i_m | kj} = \sum_{\mu=1}^m a_{i_1 \dots i_{\mu-1} \lambda i_{\mu+1} \dots i_m} R^{\lambda}_{i\mu jk}, \quad (\text{A4.10})$$

in which R^{λ}_{ijk} is the Riemann-Christoffel^(a8) or curvature tensor, and may be reduced by subsequent calculation to the form

$$(c - \frac{1}{4} a^{i,j}_{i|j})_{|\mu} = 0, \quad (\text{A4.11})$$

when the result follows precisely as above.

Theorem 4.2: Quantization of bilinear momentum observables based upon correspondence between positive classical and quantum forms.

If the bilinear momenta have the general form

$$Q_o(a^{ij}p_i p_j) = (-i\hbar)^2 (a^{ij}\delta_i \delta_j + a^{ij}_{|j} \delta_i + \alpha a^{ij}_{|ij} + \beta a^{ij}_{|i|j}) , \quad (A4.12)$$

in which the quantities α and β are (universally fixed but unknown) real constants, and if further the quantization is such that positive bilinear momenta correspond to positive quantum operators; then $\alpha = \beta = 0$.

Proof: This follows by combining the deduced inequalities obtained from the following four special cases.

example 1: On the manifold $(-1,1)$ with the usual (unit) metric the observable $A = x^2 p^2$.

Substituting from the general expression (A4.12) above we obtain as the (necessarily positive) quantum analogue of A the expression

$$Q_o(A) = (-i\hbar)^2 (x^2 D^2 + 2xD + 2(\alpha+\beta)) , \quad (A4.13)$$

from which upon noting that the operator $(-i\hbar)^2 (a^{ij}\delta_i \delta_j + a^{ij}_{|j} \delta_i)$ is positive whenever $a^{ij}p_i p_j$ is positive, we may deduce that $\alpha + \beta \geq 0$.

example 2: On the manifold $(0,\pi)$ with the usual metric the observable $A = (\sin x)p^2$.

Analogously to the method of example 1 above we deduce $\alpha + \beta \leq 0$.

example 3: On the Euclidean space $(-1,1) \times (-1,1)$ with the usual metric, the observable $A = (p_x + x p_y)^2$.

As above we obtain that $\beta \geq 0$.

example 4: On the manifold $(0, \pi) \times \mathbb{R}$ with the usual metric the
 observable $A = (p_x + (\sin^{\frac{1}{2}} x) p_y)^2$.

Deduce $\beta \leq 0$.

Appendix 5: An Illustration of the Proposed Quantization Scheme.

We develop in this appendix the detailed theory referred to in §5 of the third chapter, and begin by evaluating the coefficients in the natural decompositions of $Q_0(x^n p^n)$, for which purpose we require a series of technical lemmata.

$$\text{Lemma 5.1: } (xD)^n = \sum_{k=0}^n (-\tfrac{1}{2})^{n-k} \binom{n}{k} (xD+\tfrac{1}{2})^k, \quad n \geq 0, \quad (\text{A5.1})$$

D denoting the operation of differentiation, upon \mathcal{R} with the usual metric, with respect to the global Cartesian coordinate x .

Proof: By induction. The result being trivial when $n=0$, we need only consider the general inductive argument which is immediate from the following identities:

$$\begin{aligned} (xD)^n &= (xD)(xD)^{n-1} = (xD+\tfrac{1}{2}) \sum_{k=0}^{n-1} (-\tfrac{1}{2})^{n-1-k} \binom{n-1}{k} (xD+\tfrac{1}{2})^k \quad (\text{A5.2}) \\ &\quad - \tfrac{1}{2} \sum_{k=0}^{n-1} (-\tfrac{1}{2})^{n-1-k} \binom{n-1}{k} (xD+\tfrac{1}{2})^k \\ &= \sum_{k=0}^n (-\tfrac{1}{2})^{n-k} \left[\binom{n-1}{k-1} + \binom{n-1}{k} \right] (xD+\tfrac{1}{2})^k = \sum_{k=0}^n (-\tfrac{1}{2})^{n-k} \binom{n}{k} (xD+\tfrac{1}{2})^k. \end{aligned}$$

$$\text{Lemma 5.2: } x^n D^n = \sum_{\ell=1}^{n+1} S_n^\ell (xD)^\ell, \quad (\text{A5.3})$$

where S_n^ℓ is a Stirling number of the first kind.

Proof: see Jordan^(a9).

$$\text{Lemma 5.3: If } Q_0(x^n p^n) = \sum_{j=0}^n (-i\hbar)^{n-j} \beta_j^n Q_0^j(xp), \text{ then}$$

$$\beta_j^{2n} = \sum_{k=0, j-n-1}^n \sum_{\ell=1, j}^{n+k+1} \binom{n}{k} \frac{(2n)!}{(n+k)!} (-\tfrac{1}{2})^{\ell-j} S_{n+k}^\ell, \quad (\text{A5.4})$$

$$\beta_j^{2n+1} = \sum_{k=0, j-n-1}^n \sum_{\ell=1, j}^{n+k+1} [\binom{n+1}{k} - \frac{1}{2} \binom{n}{k}] \frac{(2n+1)!}{(n+k)!} (-\frac{1}{2})^{\ell-j} S_{n+k}^{\ell} \quad (\text{A5.5})$$

in which the lower limits of summation are taken to be the larger of the pair of options.

Proof: Consider firstly the case of β_j^{2n} , the even case. We have that by definition

$$\begin{aligned} Q_0(x^{2n}_p x^{2n}) &= \equiv_0(x^{2n}_p x^{2n}) = (-i\hbar)^{2n} D^n x^{2n} D^n \\ &= \sum_{k=0}^n (-i\hbar)^{2n} \binom{n}{k} (D^{n-k} x^{2n}) D^{n+k}, \end{aligned} \quad (\text{A5.6})$$

which yields that

$$Q_0(x^{2n}_p x^{2n}) = (-i\hbar)^{2n} \sum_{k=0}^n \binom{n}{k} \frac{(2n)!}{(n+k)!} x^{n+k} D^{n+k}, \quad (\text{A5.7})$$

and hence finally, by substitution from lemma 5.2, that

$$Q_0(x^{2n}_p x^{2n}) = (-i\hbar)^{2n} \sum_{k=0}^n \sum_{\ell=1}^{n+k+1} \binom{n}{k} \frac{(2n)!}{(n+k)!} S_{n+k}^{\ell} (xD)^{\ell}. \quad (\text{A5.8})$$

Hence, noting that $Q_0(xp) = (-i\hbar)(xD + \frac{1}{2})$ and the result of lemma 5.1, we obtain the triple sum

$$Q_0(x^{2n}_p x^{2n}) = \sum_{k=0}^n \sum_{\ell=1}^{n+k+1} \sum_{j=0}^{\ell} (-i\hbar)^{2n-j} \binom{n}{k} \frac{(2n)!}{(n+k)!} S_{n+k}^{\ell} (-\frac{1}{2})^{\ell-j} \binom{\ell}{j} Q_0^j(xp), \quad (\text{A5.9})$$

which, upon comparison with the standard form and rearrangement of the order of summation, yields the required result for β_j^{2n} .

Consider finally the case of β_j^{2n+1} , the odd case. We have that by definition

$$Q_0(x^{2n+1}_p x^{2n+1}) = (-i\hbar)^{2n+1} D^n \frac{1}{2} \{x, D\} D^n \quad (\text{A5.10})$$

which yields after simplification that

$$Q_0(x^{2n+1}_p x^{2n+1}) = (-i\hbar)^{2n+1} \sum_{k=0}^{n+1} [\binom{n+1}{k} - \frac{1}{2} \binom{n}{k}] \frac{(2n+1)!}{(n+k)!} x^{n+k} D^{n+k}, \quad (\text{A5.11})$$

$$Q_0(x^{2n+1} p^{2n+1}) = \sum_{k=0}^{n+1} \sum_{\ell=1}^{n+k+1} \sum_{j=0}^{\ell} (-i\hbar)^{2n+1-j} \left[\binom{n+1}{k} - \frac{1}{2} \binom{n}{k} \right] \frac{(2n+1)!}{(n+k)!} S_{n+k}^{\ell} (-\frac{1}{2})^{\ell-j} Q_0^j(xp). \quad (\text{A5.12})$$

Finally, rearranging the order of summation and comparing the resultant expression with the standard expression in β_k^{2n+1} , we obtain the required expression (A5.5) above.

$$\text{Lemma 5.4: } \beta_{j+1}^{2n+1} = \beta_j^{2n} \quad n \in \mathbb{N} \setminus \{0\}, j \in \mathbb{N} \setminus \{0\}; \quad (\text{A5.13})$$

$$\beta_j^{2n} = \frac{1}{2\pi i} \oint (x+n)!/(x-n)! (x+\frac{1}{2})^{-(1+j)} dx, \quad (\text{A5.14})$$

where the contour is any which contains the singularity at $x = -\frac{1}{2}$.

Proof: Examination of the series expressions (A5.4), (A5.5) for β_j^n yields that they each contain the common inner summation

$$\sum_{\ell=1, j}^{n+k+1} (-\frac{1}{2})^{\ell} \binom{\ell}{j} S_{n+k}^{\ell}. \quad (\text{A5.15})$$

The residue and binomial theorems now yield that

$$S_{n+k}^{\ell} = \frac{1}{2\pi i} \oint \frac{x!}{(x-n-k)!} \frac{1}{x^{\ell+1}} dx, \quad (\text{A5.16})$$

and that

$$x^j/(1-x)^{j+1} = \sum_{\ell=j}^{\infty} \binom{\ell}{j} x^{\ell}, \quad (\text{A5.17})$$

from which the inner summation (A5.15) may be written as

$$\frac{1}{2\pi i} \oint 2x!/[(x-n-k)! (-1)^j (1+2x)^{j+1}] dx. \quad (\text{A5.18})$$

We now address the problem of finding contour integral expressions for the coefficients β_j^n , and begin by discussing the even case. Substitution of (A5.18) for the inner summation of β_j^{2n} in (A5.4) above yields that

$$\begin{aligned}
\beta_j^{2n} &= \frac{2^{j+1}(2n)!}{2\pi i} \oint \frac{dx}{(1+2x)^{j+1}} \sum_{k=0, j-n-1}^n \binom{x}{n+k} \binom{n}{k} \quad (A5.19) \\
&= \frac{(2n)!}{2\pi i} \oint \frac{dx}{(x+\frac{1}{2})^{j+1}} \sum_{k=0, j-n-1}^n \binom{x}{n+k} \binom{n}{k} .
\end{aligned}$$

Now if $k < j-n-1$ then $\binom{x}{n+k}$ is a polynomial of degree less than $n+j-n-1=j-1$, and hence makes no contribution to the contour integral, so that the inner sum may range in all cases from 0 to n thus yielding, upon noting the identity

$$\binom{n+x}{2n} = \sum_{k=0}^n \binom{x}{n+k} \binom{n}{k} , \quad (A5.20)$$

itself demonstrated by contour integral methods, that

$$\beta_j^{2n} = \frac{1}{2\pi i} \oint \frac{(x+n)!}{(x-n)!} (x+\frac{1}{2})^{-(1+j)} dx . \quad (A5.21)$$

Finally, for the odd case, substitution into the expression (A5.5) yields the expression

$$\beta_j^{2n+1} = \frac{2^{j+1}(2n+1)!}{2\pi i} \oint \frac{dx}{(1+2x)^{j+1}} \sum_{k=0, j-n-1}^{n+1} \left[\binom{n+1}{k} - \frac{1}{2} \binom{n}{k} \right] \binom{x}{n+k} , \quad (A5.22)$$

which, upon noting the identity

$$\binom{n+1+x}{2n+1} - \frac{1}{2} \binom{n+x}{2n} = \sum_{k=0}^n \left(\binom{n+1+x}{2n+1} - \frac{1}{2} \binom{n+x}{2n} \right) , \quad (A5.23)$$

ultimately yields the result

$$\beta_j^{2n+1} = \frac{1}{2\pi i} \oint \frac{(x+n)!}{(x-n)!} \frac{1}{(x+\frac{1}{2})^j} dx = \beta_{j-1}^{2n} , \quad (A5.24)$$

as was required.

$$\text{Lemma 5.5: } \beta_j^{2n} = \sum_{k=j}^{2n} S_{2n}^k \binom{k}{j} (n-\frac{1}{2})^{k-j} . \quad (A5.25)$$

Proof: Noting the contour integral expression for S_{2n}^k (A5.16) and substituting this into the right-hand expression (A5.26), we

obtain

$$\frac{1}{2\pi i} \oint \frac{x!}{(x-2n)!} \sum_{k=j}^n \binom{k}{j} (n-\frac{1}{2})^{k-j} (1/x^{k+1}) dx, \quad (\text{A5.26})$$

which, upon our noting that the upper limit of summation may be extended to infinity without altering the residue, and upon our substitution from the identity

$$x^j / (1-x)^{j+1} = \sum_{\ell=j}^{\infty} \binom{\ell}{j} x^{\ell}, \quad (\text{A5.27})$$

yields the equivalent form

$$\begin{aligned} & \frac{1}{2\pi i} \oint \frac{x!}{(x-2n)!} \frac{1}{x} \frac{[(n-\frac{1}{2})/x]^j}{[1 - (n-\frac{1}{2})/x]^{j+1}} (n-\frac{1}{2})^{-j} dx \\ &= \frac{1}{2\pi i} \oint \frac{x!}{(x-2n)!} \frac{dx}{[x-n+\frac{1}{2}]^{j+1}}. \end{aligned} \quad (\text{A5.28})$$

Finally setting $y = x-n$ we obtain

$$\frac{1}{2\pi i} \oint \frac{(y+n)!}{(y-n)!} \frac{dy}{(y+\frac{1}{2})^{j+1}} = \beta_j^{2n} \quad (\text{A5.29})$$

as was required.

Theorem 5.6: On the decomposition of the operators $Q_0(x^n p^n)$, $n \in N$.

The operators $Q_0(x^n p^n)$, $n \in N$, satisfy an expansion of the form

$$Q_0(x^n p^n) = \sum_{j=0}^n (-i\hbar)^{n-j} \beta_j^n Q_0^j(xp), \quad (\text{A5.30})$$

in which the coefficients β_j^n are presented by the system

$$\beta_j^{2\ell} = \beta_{j+1}^{2\ell+1} = \sum_{k=j}^{2\ell} S_{2\ell}^k \binom{k}{j} (\ell-\frac{1}{2})^{k-j}, \quad \ell \in N \cup \{0\}, \quad j \in [0, 2\ell], \quad (\text{A5.31})$$

and in particular satisfy the conditions

$$\beta_{2j+1}^{2\ell} = \beta_{2j}^{2\ell-1} = 0, \quad \ell \in N, \quad j \in [0, 2\ell]. \quad (\text{A5.32})$$

Proof: Of these results all, else (A5.32), are proved in the

preceding lemmata, (A5.32) following immediately from the

symmetry of $Q_0(x^n p^n)$ but may be checked by explicit calculation based upon the contour integral (A5.29).

Theorem 5.7: On the expansion of $Q_0(\sin xp)$.

The observable $Q_0(\sin xp)$ has the formal expansion

$$Q_0(\sin xp) = \sin(2/\hbar \sinh^{-1}(\hbar/2) Q_0(xp)) . \quad (A5.33)$$

Proof: We have by hypothesis that

$$Q_0(\sin xp) = Q_0\left(\sum_{n=0}^{\infty} (-1)^n x^{2n+1} p^{2n+1} / (2n+1)!\right) = \sum_{n=0}^{\infty} (-1)^n Q(x^{2n+1} p^{2n+1}) / (2n+1)! \quad (A5.34)$$

in which the expressions for $Q(x^{2n+1} p^{2n+1})$ are as above.

Hence, substituting from lemma 5.3 and lemma 5.4, we may deduce that

$$Q_0(\sin xp) = \frac{1}{2\pi i} \oint \sum_{n=0}^{\infty} \sum_{k=0}^n \frac{(-1)^k \hbar^{2n}}{(2n+1)!} \frac{(x+n)!}{(x-n)!} \frac{Q_0^{2k+1}(xp)}{\hbar^{2k} (x+\frac{1}{2})^{2k+1}} dx . \quad (A5.35)$$

Let us now turn our attention to the evaluation of the above double sum, and first note that the quantities $\beta_{2k+1}^{2n+1} = 0$, $k > n$, so that the k -index may be extended to infinity without altering the value of the sum. This observation results in the following (formal) identities:

$$\begin{aligned} Q_0(\sin xp) &= \frac{Q_0(xp)}{2\pi i} \oint \sum_{n=0}^{\infty} \frac{(x+n)!}{(x-n)!} \frac{\hbar^{2n}}{(2n+1)!} \sum_{k=0}^{\infty} \frac{(-1)^k Q_0^{2k}(xp)}{\hbar^{2k} (x+\frac{1}{2})^{2k+1}} \\ &= \frac{Q_0(xp)}{2\pi i} \oint \sum_{n=0}^{\infty} \frac{(x+n)!}{(x-n)!} \frac{\hbar^{2n}}{(2n+1)!} \frac{(x+\frac{1}{2})}{(x+\frac{1}{2})^2 + Q_0^2(xp)/\hbar^2} . \end{aligned} \quad (A5.36)$$

Now set $y = x + \frac{1}{2}$ to obtain

$$Q_0(\sin xp) = \frac{Q_0(xp)}{2\pi i} \oint \sum_{n=0}^{\infty} \frac{(y-\frac{1}{2}+n)! \hbar^{2n}}{(y-\frac{1}{2}-n)! (2n+1)!} \frac{y}{y^2 + Q_0^2(xp)/\hbar^2} dy , \quad (A5.37)$$

and consider the remaining summation, which after some

rearrangement may be expressed in terms of the hypergeometric function^(a11)

$$F(a, b, c, x) = \sum_{n=0}^{\infty} \frac{(a+n-1)!(b+n-1)!(c-1)!x^n}{(a-1)!(b-1)!(c+n-1)!n!}, \quad (A5.38)$$

as

$$\sum_{n=0}^{\infty} \frac{(y+n-\frac{1}{2})!\hbar^{2n}}{(y-n-\frac{1}{2})!(2n+1)!} = F(\frac{1}{2}+y, \frac{1}{2}-y, \frac{3}{2}, -\hbar^2/4). \quad (A5.39)$$

Reference to standard tables^(a12) yields the identity

$$F(\frac{1}{2}+b, \frac{1}{2}-b, \frac{3}{2}, \sin^2 x) = \sin(2bx)/(2b\sin x), \quad (A5.40)$$

from which we obtain the final contour integral expression

$$Q_0(\sin xp) = \frac{Q_0(xp)}{2\pi i \hbar} \oint \sinh(2\mu \sinh^{-1} \hbar/2) / (y^2 + Q_0^2(xp)/\hbar^2) dy. \quad (A5.41)$$

Thus employing the residue theorem we obtain

$$\begin{aligned} Q_0(\sin xp) &= \hbar^{-1} Q_0(xp) [(2iQ_0(xp)/\hbar)^{-1} \sinh(2i\hbar^{-1} Q_0(xp) \sinh^{-1}(\hbar/2)) \\ &\quad - (2iQ_0(xp)/\hbar)^{-1} \sinh(-2i\hbar^{-1} Q_0(xp) \sinh^{-1}(\hbar/2)) \\ &= \sin(Q_0(xp) (\hbar/2)^{-1} \sinh^{-1}(\hbar/2)), \end{aligned} \quad (A5.42)$$

as was required.

Theorem 5.8: On the expansion of $Q_0(\cos xp)$.

The observable $Q_0(\cos xp)$ has the formal expansion

$$Q_0(\cos xp) = (1+\hbar^2/4)^{-\frac{1}{2}} \cos(2/\hbar \sinh^{-1}(\hbar/2) Q_0(xp)). \quad (A5.43)$$

Proof: Proceeding exactly as for $Q_0(\sin xp)$ deduce that

$$Q_0(\cos xp) = \frac{1}{2\pi i} \oint \sum_{n=0}^{\infty} \frac{(y+n-\frac{1}{2})!\hbar^{2n}}{(y-n-\frac{1}{2})!(2n)!} \frac{y}{y^2 + Q_0^2(xp)/\hbar^2} dy, \quad (A5.44)$$

and obtain the identity

$$\sum_{n=0}^{\infty} \frac{(y+n-\frac{1}{2})! \kappa^{2n}}{(y-n-\frac{1}{2})! (2n)!} = F(y+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}, -\frac{\kappa^2}{4}). \quad (\text{A5.45})$$

These, together with the further identity^(a13)

$$F(\frac{1}{2}+b, \frac{1}{2}-b, \frac{1}{2}, \sin^2 x) = \cos(2bx)/\cos x, \quad (\text{A5.46})$$

yield the final contour integral expression

$$Q_0(\cos xp) = (1+\kappa^2/4)^{-\frac{1}{2}} \oint \frac{\cosh(2y \sinh^{-1}(\kappa/2))}{(y^2 + Q_0^2(xp)/\kappa^2)} y dy, \quad (\text{A5.47})$$

from which the result follows by the residue theorem.

note: The remaining results (70) of theorem 9 of chapter 3 follow from the expressions for $Q_0(\sin xp)$ and $Q_0(\cos xp)$ by re-expressing $\cosh x$ as $\cos ix$ etc.

This completes the fifth appendix.

References to the Appendices
of
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- a1: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry...",
second edition, Wiley (1964), §7, pp16-17.
- a2: Synge J.L. and Schild A.: "Tensor Calculus", University of Toronto
Press (1949), §2.5, pp51-54.
- a3: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry...",
second edition, Wiley (1964), §40, p.97.
- a4: Synge J.L. and Schild A.: "Tensor Analysis", University of Toronto
Press (1949), §6.1, pp193-194.
- a5: Spiegel M.R.: "Theory and Problems of Advanced Mathematics...",
McGraw-Hill (1971), Chapt.13, pp289-290.
- a6: Abramowitz M. ed.: "Handbook of Mathematical Functions...",
National Bureau of Standards (1964), §24, p.822.
- a7: Sokolnikoff I.S.: "Tensor Analysis and Applications to Geometry...",
second edition, Wiley (1964), §36, p.89.
- a8: Coburn N.: "Vector and Tensor Analysis", Macmillan (1955), §54,
pp239-241.
- a9: Jordan C.: "Calculus of Finite Differences", second edition,
Chelsea Publishing Company (1950), §69, p.197.
- a10: Jordan C.: "Calculus of Finite Differences", second edition,
Chelsea Publishing Company (1950), §50, p.142.
- a11: Erdelyi A., director: "Higher Transcendental Functions", Volume 1,
McGraw-Hill (1953), §2.1, p.56.
- a12: Erdelyi A., director: "Higher Transcendental Functions", Volume 1,
McGraw-Hill (1953), §2.8, p.101.
- a13: Erdelyi A., director: "Higher Transcendental Functions", Volume 1,
McGraw-Hill (1953), §2.8, p.101.

Bibliography

Bibliography

- 1: Abraham R. and Marsden J.E.: "Foundations of Mechanics", second edition, Benjamin/Cummings (1978).
- 2: Abramowitz M. ed.: "Handbook of Mathematical Functions...", McGraw-Hill (1971).
- 3: Aharanov Y. and Safko J.L.: "Measurement of Noncanonical Variables", Ann. Phys. 91 (1975), 279-.
- 4: Akhiezer N.I. and Glasman I.M.: "Theory of Linear Operators in Hilbert Space", volume 1, Frederick Ungar (1961).
- 5: Assimakopoulos M., Bloore F.J. and Ghobrial I.R.: "Quantization as a deformation theory", J. Math. Phys. 17 (1976), 1034-1038.
- 6: Bishop R.L. and Crittenden R.J.: "Geometry of Manifolds", Academic Press (1964).
- 7: Bloore F.J.: "Quantization on a Riemannian Manifold", Colloques Internationaux C.N.R.S., no.237, pp299-303.

Bloore F.J. and Ghobrial I.R.: "Quantum mechanical ordering problem for observables which are linear in momentum", J. Phys. A.: Math. Gen. 8 (1975), 1863-.

Bloore F.J. and Routh L.: "The Covariant Form for Quantum-Mechanical Operators which are Quadratic in Momentum", Nuovo Cimento 47B (1978), 78-84.

Bloore F.J., Assimakopoulos M. and Ghobrial I.R.: "Quantization as a deformation theory", J. Math. Phys. 17 (1976), 1034-1038.
- 8: Brickell F. and Clarke R.S.: "Differentiable Manifolds", Van Nostrand Reinhold (1970).
- 9: Britten W.E. ed.: "Lectures in Theoretical Physics", volume VIII A, Gordon and Breach (1966).
- 10: Capri A.Z.: "Self-Adjointness and Spontaneously Broken Symmetry", Am. J. Phys. 45 (1977), 823-.
- 11: Castellani L.: "Quantization Rules and Dirac's Correspondence", Nuovo Cimento 48A (1978), 359-363.

- 12: Chernoff P.: "Essential Self-Adjointness of powers of generators of hyperbolic equations", J. Funct. Anal. 12 (1973), 401-414.
- 13: Choquet-Bruhat Y., De Witt-Morette C. and Dillard-Bleick M.:
"Analysis, Manifolds and Physics", North Holland (1977).
- 14: Clark R.S. and Brickell F.: "Differentiable Manifolds", Van Nostrand Reinhold (1970).
- 15: Coburn N.: "Vector and Tensor Analysis", MacMillan (1955).
- 16: Courant R. and Hilbert D.: "Partial Differential Equations", volume 2, Interscience (1962).
- 17: Crittenden R.J. and Bishop R.L.: "Geometry of Manifolds", Academic Press (1964).
- 18: De Witt-Morette C., Choquet-Bruhat Y. and Dillard-Bleick M.:
"Analysis, Manifolds and Physics", North Holland (1977).
- 19: Dicke R.H. and Wittke J.P.: "Introduction to Quantum Mechanics", Addison-Wesley (1963).
- 20: Dillard-Bleick M., Choquet-Bruhat Y. and De Witt-Morette C.:
"Analysis, Manifolds and Physics", North Holland (1977).
- 21: Dirac P.A.M.: "Principles of Quantum Mechanics", Oxford (1958).
- 22: Eisenhart L.P.: "Riemannian Geometry", Princeton (1926).
- 23: Erdelyi A., director: "Higher Transcendental Functions", volume 1, McGraw-Hill (1953).
- 24: Ghobrial I.R. and Bloore F.J.: "Quantum mechanical ordering problem for observables which are linear in momentum", J. Phys. A.: Math. Gen. 8 (1975), 1863-.
- Ghobrial I.R., Assimakopoulos M. and Bloore F.J.: "Quantization as a deformation theory", J. Math. Phys. 17 (1976), 1034-1038.
- 25: Glasman I.M. and Akhiezer N.I.: "Theory of Linear Operators in Hilbert Space", volume 1, Frederick Ungar (1961).
- 26: Goldstein H.: "Classical Mechanics", Addison-Wesley (1972).
- 27: Guest P.B.: "The Quantization of Classical Systems", Rep. Math. Phys. 6, 99-157.

- 28: Hellwig G.: "Differential Operators of Mathematical Physics",
Addison-Wesley (1967).
- 29: Herman R.: "Yang-Mills, Kaluza-Klein, and the Einstein Programme",
Math. Sci. Press (1978).
- 30: Hilbert D. and Courant R.: "Partial Differential Equations",
volume 2, Interscience (1962).
- 31: Hunter J. and Monk D.: "Algebra and Number Systems", Blackie/
Chambers (1971).
- 32: Jordan C.: "Calculus of Finite Differences", second edition,
Chelsea Publishing Company (1950).
- 33: Kumura T.: "On the Quantization of Non-Linear Theories", Prog.
Theor. Phys. 46 (1971), 1261-1277.
- 34: Kreyzig E.: "Introductory Mathematical Statistics", Wiley (1970).
- 35: Loomis L.H. and Sternberg S.: "Advanced Calculus", Addison-Wesley
(1968).
- 36: Mackey G.W.: "The Mathematical Foundations of Quantum Mechanics",
W.A. Benjamin (1963).
- 37: Marsden J.E. and Abraham R.: "Foundations of Mechanics", second
edition, Benjamin/Cummings (1978).
- 38: McFarlane K. and Wan K.K.: "The Quantization and Measurement of
Momentum Observables", J. Phys. A: Math. Gen. (1980), in
press.
- 39: Messiah A.: "Quantum Mechanics", volume 1, North Holland (1961).
- 40: Monk D. and Hunter J.: "Algebra and Number Systems", Blackie/
Chambers (1971).
- 41: Mukunda N. and Sudarshan E.C.G.: "Classical Dynamics: A Modern
Perspective", Wiley and Sons (1974).
- 42: Naimark M.A.: "Linear Differential Operators", George G. Harrap &
Co. (1968).
- 43: Prugovecki E.: "Quantum Mechanics in Hilbert Space", Academic
Press (1971).

- 44: Roman P.: "Advanced Quantum Theory", Addison-Wesley (1965).
- 45: Routh L. and Bloore F.J.: "The Covariant Form for Quantum-Mechanical Operators which are Quadratic in Momentum", *Nuovo Cimento* 47B (1978), 78-84.
- 46: Schiff L.I.: "Quantum Mechanics", third edition, McGraw-Hill (1968).
- 47: Schild A. and Synge J.L.: "Tensor Calculus", University of Toronto Press (1966).
- 48: Segal I.E.: "Quantization of Nonlinear Systems", *J. Math. Phys.* 1 (1960), 468-488.
- 49: Sokolnickoff I.S.: "Tensor Analysis and Applications to Geometry...", second edition, Wiley (1964).
- 50: Spiegel M.R.: "Theory and Problems of Advanced Mathematics", McGraw-Hill (1971).
- 51: Sternberg S. and Loomis L.H.: "Advanced Calculus", Addison-Wesley (1968).
- 52: Sudarshan E.C.G. and Mukunda N.: "Classical Dynamics: A Modern Perspective", Wiley and Sons (1974).
- 53: Synge J.L.: "Relativity, the General Theory", North Holland (1971).
Synge J.L. and Schild A.: "Tensor Calculus", University of Toronto Press (1966).
- 54: Taraviras S. and Underhill J.: "Weyl Quantization on a Sphere", *Lecture Notes in Physics* 50, Group Theoretical Methods in Physics, Fourth International Colloquium, Nijmegen 1975, Springer-Verlag (1976), pp210-216.
- 55: Temple G.: "The Fundamental Paradox of Quantum Theory", *Nature* (1935), 957.
- 56: Underhill J. and Taraviras S.: "Weyl Quantization on a Sphere", *Lecture Notes in Physics* 50, Group Theoretical Methods in Physics, Fourth International Colloquium, Nijmegen 1975, Springer-Verlag (1976), pp210-216.

- Underhill J.: "Quantization on a Manifold with Connection", J. Math. Phys. (1977) 19 1932-1935.
- 57: Van Hove L.: "Sur certaines representations unitaires d'un groupe infini de transformations", Mem. de l'Acad. Roy. de Belgique (Classe des Sci.) 26, 61-102.
- 58: Varadarajan V.S.: "Geometry of Quantum Theory", volume 2, Van Nostrand Reinhold (1970).
- 59: Viazminsky C. and Wan K.K.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977), 1030-1044.
- Viazminsky C. and Wan K.K.: "Lie algebra and the quantization of the Hamiltonian", J. Phys. A: Math. Gen. 12 (1979), 643-647.
- 60: Wan K.K. and Viazminsky C.: "Quantization in Spaces of Constant Curvature", Prog. Theor. Phys. 58 (1977), 1030-1044.
- Wan K.K. and Viazminsky C.: "Lie algebra and the quantization of the Hamiltonian", J. Phys. A: Math. Gen. 12 (1979), 643-647.
- Wan K.K. and McFarlane K.: "The Quantization and Measurement of Momentum Observables", J. Phys. A: Math. Gen. (1980), in press.
- 61: Weinstock R.: "Calculus of Variations", McGraw-Hill (1952).
- 62: Weyl H.: "Theory of Groups and Quantum Mechanics", second edition, Dover (1931).
- 63: Wittke J.P. and Dicke R.H.: "Introduction to Quantum Mechanics", Addison-Wesley (1963).